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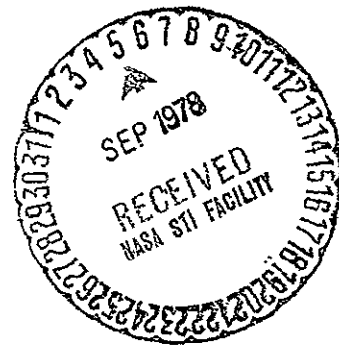
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MATHEMATICAL AND COMPUTATIONAL STUDIES OF EQUILIBRIUM

CAPILLARY FREE SURFACES

by Norman Albright, Nai-Fu Chen,
Paul Concus, and Robert Finn

We present here the results of our mathematical and computational studies of equilibrium capillary free surfaces that have been carried out over the past few years. These studies center on the equation

$$(1) \quad \frac{\partial}{\partial x} \left(\frac{1}{W} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{1}{W} \frac{\partial u}{\partial y} \right) = \kappa u + 2H ,$$

$$W = \left[1 + \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 \right]^{1/2} ,$$

which is satisfied by the single-valued height $u(x,y)$ of a liquid-vapor free surface in Laplace equilibrium (mechanical balance between gravitational and surface forces). The gravitational force is assumed to be uniform and directed vertically, and in (1) the quantity $\kappa = \rho g / \sigma$ is the capillary constant, with ρ the difference in densities between the vapor and liquid phases, g the acceleration field -- positive, negative, or zero -- and σ the liquid-vapor surface tension; $2H$ is a constant, which is determined for a given problem, usually indirectly, by constraints such as container shape, liquid volume, and contact angle.

Our studies have pursued several directions, each of which is discussed independently in a self-contained manner in Appendices I to V.

In Appendix I, the general question is considered of whether a wetting liquid always rises higher in a small capillary tube than in a larger one, when both are dipped vertically into an infinite reservoir. For this situation, the height of the free surface

satisfies (1), with $H=0$ when $u(x,y)$ is measured vertically upward from the reservoir level $u=0$, and the contact angle condition

$$(2) \quad \frac{1}{W} \frac{\partial u}{\partial n} = \cos \gamma$$

is imposed at the tube walls, where $\partial u / \partial n$ is the derivative of u with respect to the outer directed normal to the wall and γ is the contact angle (between 0 and $\pi/2$ for a wetting liquid).

It is generally known that if a given circular tube T_0 , dipped into a reservoir, is replaced by a concentric one T_1 of smaller diameter, then the liquid-vapor free surface $u_1(x,y)$ in T_1 is at all points higher than was the (original) surface $u_0(x,y)$ in T_0 . We have proved that for circular T_0 this is still the case, no matter what the placement or cross section of T_1 , provided only that it lies interior to the space originally occupied by T_0 .

When the larger tube T_0 is not circular, the situation can be very different. In chapter I it is proved, by example, that if $\gamma \neq 0$ there exist configurations for which the volume (and hence the average rise height) of liquid lifted by T_0 over the cross section of T_1 exceeds that lifted by T_1 . For the configurations considered in Appendix I the cross section of the larger tube has a corner, however the result can be obtained even if corners are rounded so that both tubes are smooth and convex. We are continuing to pursue this question beyond the initial investigation reported here.

In Appendix II is initiated an analytical investigation of the relationship between the family of solutions of (1) corresponding to rotationally symmetric pendent liquid drops and the singular solution, corresponding to an infinite spike of liquid extending downward to infinity, whose existence we have proved previously. For these surfaces, $\kappa < 0$, and $H=0$ for u measured from the free plane reference level, so that the rotationally symmetric form of (1), suitably normalized, is

$$\frac{1}{r} \frac{d}{dr} \left[\frac{r \, du/dr}{[1 + (du/dr)^2]^{1/2}} \right] = -u \quad ,$$

or, in parametric form,

$$\begin{aligned} \frac{dr}{ds} &= \cos \psi \\ (4) \quad \frac{du}{ds} &= \sin \psi \\ \frac{d\psi}{ds} &= -u - \frac{\sin \psi}{r} \quad . \end{aligned}$$

Here s is arc length, r is the distance from the axis of symmetry, and ψ is the angle made by a tangent to a vertical section with the r axis.

For the pendent-drop family of solutions, the initial conditions are

$$(5) \quad r(0) = 0, \quad u(0) = u_0 < 0, \quad \psi(0) = 0 \quad ,$$

whereas for the singular solution $u \sim -1/r$ as $r \rightarrow 0$. We prove in Appendix II that for u_0 sufficiently small in magnitude the solutions of (4,5) can be expressed as a single-valued function $u = u(r)$ for all r , i.e. no verticals can occur.

For larger values of $|u_0|$ we prove that no such global representation is possible. (Numerical computations give $u_0 \approx -2.57$ as the critical value for which a vertical first appears.)

For very large values of $|u_0|$ the solutions of (4,5) are shown to have near their vertex the general form of a succession of circular arcs joined near the vertical axis by small arcs of large curvature. However, their continuation eventually projects simply on $u=0$ and continues in an oscillatory manner to infinity. Our analytical estimates for large $|u_0|$ are obtained using a technique that compares the solution surface with surfaces of constant mean curvature that are generated by the roulades of an ellipse.

We conjecture that as $|u_0| \rightarrow \infty$ the pendent-drop solutions converge, uniformly in any $|u| < \hat{u} < \infty$, to the singular solution, which has a simple projection on $u=0$. If the pendent-drop solutions are considered from the point of view of their global embedding in the manifold of all formal solutions of the equations, then the vertex of the drops appear as a transition point marking a change in qualitative appearance. It is conjectured that the only global solution of (4) without double points, in this extended sense, is the singular solution.

Our study reported in Appendix II has been extended, and will appear in its completed form as reference [18] of that chapter. These studies of equilibrium pendent liquid drops are intended as a first step in approaching the question of stability of such drops.

The studies in Appendices III and IV are computational ones that center on developing and comparing numerical methods for solving (1,2) for $\kappa > 0$ in domains that are noncircular -- i.e., finding equilibrium free surfaces in vertical cylinders with noncircular cross sections for the case of downward-acting gravity. (If $\kappa \leq 0$, existence or uniqueness may fail.) Without a loss of generality, only wetting liquids ($0 \leq \gamma < \pi/2$) are considered. Of particular interest are the difficulties that can arise for the case of a domain containing corners.

The model problem considered in Appendix III is that of a cylinder with a square cross section. Because of symmetry, only one-quarter of the square is taken as the domain for the study, and we place on the domain a uniform square mesh, obtaining on it a corresponding discretization of (1,2). We investigate extensions of the block successive overrelaxation-Newton method and of the generalized conjugate gradient method for obtaining the solution of the discrete problem. Both methods are found to be satisfactory for obtaining accurate solutions for $\kappa \geq 0$ for all cases in which the solution of (1,2) is bounded, although, at least for the model problem, the generalized conjugate gradient method is found to be more efficient and robust.

As we have proved earlier, if $\alpha + \gamma < \pi/2$, where 2α is the interior angle at a corner of the cylinder cross-section (for the square $\alpha = \pi/4$),

the solution is unbounded at the vertex, the asymptotic behavior near the vertex being given by

$$(5) \quad v(\rho, \theta) = [\cos\theta - (k^2 - \sin^2\theta)^{1/2}]/(k\rho) , \quad k = \sin\alpha \sec\gamma ,$$

where (ρ, θ) are polar coordinates centered at the vertex, with θ measured from the interior angle bisector. Thus special numerical methods are needed in this case to obtain an accurate numerical solution.

The methods we investigate in Appendix III are based on deleting a neighborhood of the singular corner from the numerical domain and using (5) in this neighborhood. The normal derivative of the asymptotic solution $v(\rho, \theta)$ provides the required boundary condition for the numerical problem, and the resulting solution height is then matched at the interface. In choosing the position of the interface one must strike a balance between keeping it close enough to the vertex so that the asymptotic representation is accurate over the deleted domain and keeping it far enough from the vertex so that the discretization in the numerical domain can represent the steep gradients near the corner adequately.

In an attempt to overcome this difficulty, we investigate the possibility of overlapping the asymptotic and numerical solutions over part of the domain. We find that such an attempt to improve the asymptotic solution by numerical means is not fruitful, in essence because of the steep gradients of the solution.

From our experiments we conclude that the technique of deleting a small neighborhood of the corner from the numerical domain can succeed

in yielding a sufficiently accurate solution, particularly away from the corner. In fact, the solution over the bulk of the interior of the square is rather insensitive to changes in the position of the interface between the deleted and numerical domains.

For reasons given in Appendix III, we find it desirable (a) that the interface should be chosen to be a level curve of (3) (a circular arc intersecting the edges of the square with angle γ), (b) that it be taken close to the singularity corner, (c) that a higher-order discretization, a mesh refinement, or other numerical method be used in the numerical domain, at least locally near the interface, to represent the steep gradients adequately. The computer programs prepared in connection with the study in Appendix III were written primarily for a uniform square mesh and were not sufficiently general to permit inclusion of the above features. These are examined to some extent in Appendix IV.

In Appendix IV, discretizations of (1,2) are solved on irregularly shaped domains using JASON, a general-purpose program for solving nonlinear elliptic equations on a nonuniform quadrilateral mesh. JASON is reliable and easy to use, but is not necessarily very efficient for obtaining capillary surfaces, as it is designed for a very general class of problems. It did provide means, however, for calculating capillary surfaces in more general domains than is possible with the experimental programs of Appendix III. With it, capillary surfaces are calculated on the ellipse, on a circle with reentrant notches, and on other domains.

For the ellipse, comparisons are made between the calculated results and analytical estimates of the conditions for nonexistence of solutions of (1,2) on sufficiently curved domains in zero gravity. The calculated results are consistent with the analytical estimates, and indicate that the estimates are reasonably sharp for this case.

For the circular cylinder with reentrant notches, and for a square domain, the case for which the solution surface is unbounded at a corner is studied by means of the technique described in Appendix III. Here, it is possible to approximate more closely a level curve of (5) for the interface between the deleted and the numerical domains. The numerical results for these cases are depicted graphically.

In Appendix V, the analytical estimates for nonexistence of solutions of (1,2) on the ellipse in zero gravity are evaluated. It is found that if the ratio of the minor to major semiaxes of an ellipse is less than 0.6116, then a nontrivial critical contact angle exists such that for contact angles less than this critical one there is no solution. The critical angle estimates obtained here are the ones used in Appendix IV for the comparisons with the values observed from solving (1,2) numerically.

APPENDIX I

ON THE HEIGHT OF A CAPILLARY SURFACE

by

Paul Concus and Robert Finn

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On the Height of a Capillary Surface

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1. In the “capillary problem” one seeks to determine a surface $u(x)$ satisfying the equation

$$\operatorname{div} Tu = \kappa u, \quad Tu = \frac{1}{W} \nabla u, \quad W = \sqrt{1 + |\nabla u|^2}, \quad (1)$$

in a domain Ω , and the condition

$$\nu \cdot Tu = \cos \gamma \quad (2)$$

on $\Sigma = \partial\Omega$. Here γ is prescribed, $0 \leq \gamma \leq \pi$, $\kappa = \frac{\rho g}{\sigma}$ is the “capillarity constant”, and ν is the exterior directed normal on Σ . The symbols ρ, g, σ denote density, gravitational acceleration and surface tension (all assumed constant). For background information see, e.g., [1, 2]. In this note we assume the “contact angle” γ is constant¹, and that $\kappa > 0$, corresponding to the familiar physical situation of liquid rising in a vertical capillary tube of homogeneous composition.

M. Miranda has posed to us, informally, the question: let $\Omega_1 \subset \Omega$, and let u_1, u be solutions of (1, 2) in, respectively, Ω_1 and Ω . Is $u_1 > u$ in Ω_1 ?

2. The question is physically suggestive, in the sense one expects the rise height of liquid in a capillary tube of small section to exceed that in a tube of large section.

If $\gamma = 0$ the question has an affirmative answer, under very general hypotheses, both on the domains Ω, Ω_1 and on assumption of boundary data; this follows from the particular forms of the maximum principle given by Gerhardt [3] and by these authors [4].

A heuristic reasoning, using the methods of [4], will convince the reader that the answer is again positive in the case Σ_1 and Σ are spheres (not necessarily concentric).

If $\gamma = \pi/2$ then the unique solution of (1, 2) in any Ω is $u(x) \equiv 0$; thus an affirmative answer (in an extended sense) is obtained in this limiting case.

3. In the present note we show that in general the answer is negative, even for convex domains with smooth boundaries.

Consider the two dimensional region Ω indicated in Fig. C. In § 7 of [5] is proved the existence of a unique solution $u(x)$ of (1, 2) in Ω . We note the data γ

¹ We may assume $0 \leq \gamma \leq \frac{\pi}{2}$, as the complementary case reduces to this one by a formal transformation.

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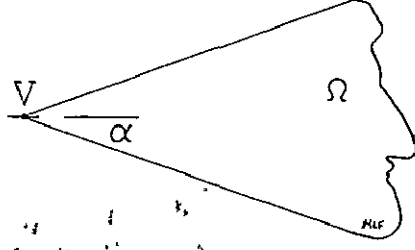


Fig. C

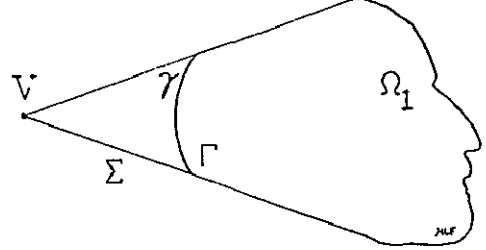


Fig. F

need not be prescribed at the corner, where the boundary angle is not defined. At all other boundary points, the data are achieved strictly and smoothly [6, 7, 8], at least if $\gamma \neq 0$.

We choose γ so that $\alpha + \gamma < \frac{\pi}{2}$. Introducing polar coordinates centered at V , we set

$$v(r, \theta) = \frac{\cos \theta - \sqrt{k^2 - \sin^2 \theta}}{\kappa k r}, \quad k = \frac{\sin \alpha}{\cos \gamma}. \quad (3)$$

There hold [4],

$$\operatorname{div} Tv = \kappa v + O(r^3) \quad (4)$$

in Ω , and

$$v \cdot Tv = \cos \gamma + O(r^4) \quad (5)$$

on the two straight segments. Further, there exists a constant C such that

$$|u - v| < C \quad (6)$$

uniformly in a neighborhood of V .

Let Ω_1 be as indicated in Fig. F. We note the circular arc Γ is a level curve for v ; since $|\nabla v| > |v_r| = \frac{1}{r}v$ becomes infinite as $r \rightarrow 0$, there follows

$$v \cdot Tv|_{\Gamma} \rightarrow 1 \quad (7)$$

as $r \rightarrow 0$. This relation is uniform on Γ .

4. We apply the divergence theorem to v in $\Omega \setminus \Omega_1$, obtaining

$$|\Sigma| \cos \gamma - \int_{\Gamma} v \cdot Tv d\sigma = \kappa \int_{\Omega \setminus \Omega_1} v dx + O(|\Sigma|^5) \quad (8)$$

by (4, 5). No contribution appears from the singularity at V , since $|Tf| < 1$ for any function f .

Repeating the procedure with v replaced by u and taking the difference of the two expressions yields

$$\left| \int_{\Gamma} v \cdot Tu d\sigma - \int_{\Gamma} v \cdot Tv d\sigma \right| \leq \kappa \int_{\Omega \setminus \Omega_1} |u - v| dx + O(|\Sigma|^5). \quad (9)$$

Hence, by (6), if $\gamma \neq 0$,

$$\int_{\Gamma} v \cdot Tu \, d\sigma > |\Gamma| \cos \gamma \quad (10)$$

if Γ is chosen sufficiently close to V .

5. Let $u_1(x)$ be the solution of (1, 2) in Ω_1 . The divergence theorem now yields

$$\int_{\Gamma} v \cdot Tu \, d\sigma - |\Gamma| \cos \gamma = \kappa \int_{\Omega_1} (u - u_1) \, dx \quad (11)$$

and we conclude, by (10), that there exists an open subset of Ω_1 in which $u > u_1$. This completes the proof of our assertion, for the particular domains considered.

6. An objection may possibly be raised, that the boundaries appearing in the above construction have singular points. However, an examination of our procedure, and of the method of construction of the function $u(x)$ in [5], shows that all corners — including the one at V — can be smoothed without affecting the qualitative result. The construction can also be effected so that $\Omega_1 \subset\subset \Omega$, and it can be repeated without essential change in any number of dimensions.

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Note Added in Proof. From Theorem 6 of [4] and known monotonicity properties of the spherically symmetric solution, one obtains an affirmative answer to Miranda's question for any Σ_1 whenever Σ is a sphere.

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APPENDIX II

ON THE SHAPE OF A PENDENT LIQUID DROP

by

Paul Concus and Robert Finn

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Abstract

A characterization is given for the most general form of a symmetric pendent liquid drop, including those situations in which equilibrium may not be stable. It is shown that for any vertex height u_0 the vertical section of the drop can be continued globally as an analytic curve, without limit sets or double points. For small $|u_0|$ it is proved the section projects simply on the axis $u=0$; for large $|u_0|$ the section is shown to have near the vertex the general form of a succession of circular arcs joined near the vertical axis by small arcs of large curvature. However, the continuation of the section eventually projects simply on $u=0$ and continues in an oscillatory manner to infinity.

It is conjectured that as $|u_0| \rightarrow \infty$ the section converges, uniformly in any $|u| < \hat{u} < \infty$, to a solution $U(r)$ with simple projection on $u=0$ and an isolated singularity at $r=0$. The (liquid drop) solutions are studied from the point of view of their global embedding in the manifold of all formal solutions of the equations. From this point of view, the vertex of the drop appears as a transition point marking a change in qualitative appearance. It is conjectured that the only global solution without double points, in this extended sense, is the singular solution $U(r)$.

The form of the outer surface of a symmetric liquid drop suspended from a circular aperture is determined by the condition that the mean curvature of the surface is proportional to the distance below a horizontal reference plane. For points near which the surface can be described by a function $u(x)$ we obtain an equation ⁽¹⁾

$$(1) \quad \frac{\partial}{\partial x_i} \left\{ \frac{u_{x_i}}{\sqrt{1 + |\nabla u|^2}} \right\} = -\kappa u + \lambda$$

for the height $u(x)$ above the plane.

Here κ is a physical constant, $\kappa > 0$ when the liquid lies above the surface, and λ is a Lagrange parameter, to be determined by the constraints.

In a specific problem the determination of λ may lead to technical difficulties. Formally, however, λ can be transformed out of (1) by adding a constant to u . In the present paper we intend to characterize all symmetric solutions for the case $\lambda=0$. A solution corresponding to given λ can then be found in this family by transforming back.

We shall also introduce the (inessential and convenient) normalization $\kappa = 1$. We then obtain, in terms of polar radius r , the equation

$$(2) \quad \left(r \frac{u_r}{\sqrt{1 + u_r^2}} \right)_r = -ru$$

for a symmetric two dimensional surface $u(r)$.

Not all surfaces that appear physically have a simple projection on a base plane, hence for a complete description the form (2) is overly restrictive. We obtain a more suitable (parametric) form of the problem if we introduce the arc length s along a vertical section of the surface interface, measured from the vertex $(0, u_0)$. We are led to the system

$$\frac{d\psi}{ds} = -u - \frac{1}{r} \sin \psi$$

$$(3) \quad \frac{du}{ds} = \sin \psi$$

$$\frac{dr}{ds} = \cos \psi$$

where ψ is the angle between a tangent to the section and the r -axis, measured counterclockwise from the positively directed axis to the tangent line.

From the point of view of general theory, one would expect a solution of (3) to be determined, at least locally, by the initial data

$$(1) \quad r(0) = 0; \quad \psi(0) = 0; \quad u(0) = u_0;$$

however, the system (3) is singular at $s = 0$, and because of this the second condition in (4) is superfluous (cf the discussion in [4]).

The question of local existence has been studied by Lohnstein [5], who established the convergence of a formal power series expansion. Alternatively, one could adapt the Picard method, as used by Johnson and Perko [6] for the capillary problem, to the case studied here. One obtains locally, by these methods, a non-parametric solution $u(r)$ of the equation (2), which we may write in the form

$$(5) \quad (r \sin \psi)_r = -ru,$$

corresponding to the (single) initial condition

$$(6) \quad u(0) = u_0.$$

The circumstance that only one initial datum is required yields an important simplification for the problem of characterizing all solutions. It suffices to describe the one-parameter family determined by u_0 , and

it is this approach we adopt in the present work.

In general, the solution $u(r; u_0)$ determined in this way cannot be continued indefinitely as solution of (5). We shall show however that for any u_0 , the function $u(r; u_0)$ can be continued as a parametric solution of (3) for all s , yielding a surface without limit sets or double points.

We shall characterize quantitatively the asymptotic form of the surface in the case $|u_0| \gg 0$, and we shall characterize qualitatively the global structure of all such surfaces.

The global behavior changes qualitatively when $|u_0|$ increases beyond a critical value. If $|u_0| \gg 0$, there is an initial range for s in which the surface looks like a succession of spheres centered on the u -axis with radius $\approx 2/|u|$. In all cases, the section can be expressed for large s in the form $u(r)$ and has an oscillatory behavior as $r \rightarrow \infty$.

If $u_0 = 0$ the unique solution of (2) is given by $u \equiv 0$. We assume throughout this paper that $u_0 < 0$; the remaining case is obtained by a simple change of sign ⁽²⁾. We are interested particularly in what happens when $u_0 \ll 0$. The resulting surfaces are then physically unstable under most conditions of everyday experience; however, the problem has an independent mathematical interest (one specific feature of which we indicate below) and probably also a physical interest for situations in which gravity forces are small compared with those of surface tension.

We have proved in [7] the existence of a particular singular solution of (2) that can be expressed in the form $U(r)$ in $0 < r < \delta$, and such that $U(r) \sim -\frac{1}{r}$ as $r \rightarrow 0$. In [8] we have presented numerical evidence suggesting that the symmetric solutions discussed above tend uniformly to $U(r)$ in any fixed region $u > A > -\infty$. A particular consequence of the analysis in the present paper will be a proof of a preliminary form of that conjecture, namely we shall show in section VI that the solutions converge asymptotically into a neighborhood of $U(r)$, the size of which can be estimated a priori and is small relative to other (local) distances.

In section VII the structure of solutions is examined from another point of view and some numerical results are presented, suggesting the types of possible global behavior. These results lead in turn to another conjecture, namely that the singular solution $U(r)$ is the only global solution (in an extended sense) that is free of double points.

We remark that we know of few other studies of the problem from a general theoretical point of view ⁽³⁾. To our knowledge the first attempt to characterize the shape of a liquid drop appears in Bashforth and Adams [10] in which a numerical procedure is developed to calculate the sectional form up to the first vertical point Thomson [11] used a geometrical method and was able to obtain a figure corresponding, in our notation, to $u_0 \approx -7$. Computational studies were greatly facilitated by development of high speed computers and related techniques, and particular cases have now been calculated with much larger $|u_0|$, see, e.g., Hida and Miura [12] and Concus and Finn [8]. Such calculations are suggestive and instructive, but they cannot provide the unifying insight of a general formal description. The present work is intended as an initial step toward that objective.

In this work we study the formal solutions of the equations and ignore the question of physical stability of the surfaces. With regard to this related matter the reader may wish to consult recent contributions by Pitts [13, 14] and by Hida and Miura [12], where also further references can be found.

The central difficulty in the general study of the solutions of (2) lies in the failure of the maximum principle. In the particular situation studied here, a residue of this principle remains, permitting us to compare the solutions with those of a simpler equation. This circumstance, in conjunction with elementary formal manipulation of the equation, provides the central tool in our investigation. We proceed in a succession of steps, most of which are elementary and immediate; when taken together, however, they yield the requisite characterization.

We remark that the comparison technique has proved effective also in other (related) contexts, and has led in particular to new information on the behavior of solutions of (2) near isolated singular points, see,

e. g., [15].

The latter author wishes to thank J. Serrin and J. Spruck for a number of stimulating conversations.

I The case of small $|u_0|$.

We shall prove :

Theorem 1 : If, in the initial value problem (5, 6) there holds ⁽⁴⁾
 $u_0 \geq -2$, then the solution can be continued as a (nonparametric) solution of the equation

$$(2) \quad \left(\frac{ru_r}{\sqrt{1+u_r^2}} \right)_r = -ru$$

for all $r > 0$. It has an infinity of zeros. For any two successive extrema r_a, r_b of $u(r)$ there holds $|u(r_b)| < |u(r_a)|$. Asymptotically as $u_0 \rightarrow 0$ the first zero r_0 is the first zero of the Bessel function $J_0(r)$, $r_0 \sim 2.405$.

We study first the portion of the trajectory preceding the first zero, and we note that (2) is equivalent to (5) on any interval on which $|u_r| < \infty$.

II : Let $u(r)$ satisfy (5) in $0 < r < R$ and (6) at $r = 0$. Then ⁽⁵⁾
 $\sin \Psi(0) = 0$.

Proof: Integrating (5) from $\epsilon > 0$ to r , we find

$$r \sin \Psi - \epsilon \sin \Psi(\epsilon) = - \int_{\epsilon}^r \rho u d\rho,$$

hence, using (6),

$$(7) \quad \sin \Psi = \frac{u_r}{\sqrt{1+u_r^2}} = - \frac{1}{r} \int_0^r \rho u d\rho$$

from which we conclude $\lim_{r \rightarrow 0} u_r(r) = 0$. Hence there exists

$$u_r(0) = \lim_{r \rightarrow 0} \frac{u(r) - u_0}{r} = \lim_{r \rightarrow 0} \frac{1}{r} \int_0^r u_r(\tau) d\tau = 0.$$

Iii Let $u(r)$ satisfy (5) in $0 < r < R$ and (6) at $r = 0$. If $u(r) < 0$ in $0 < r < R$, then $\sin \Psi > 0$ in this interval.

The proof is contained in (7).

It follows in particular that $u(r) \rightarrow u_R \leq 0$ as $r \rightarrow R$, that $\sin \Psi_R = \lim_{r \rightarrow R} \sin \Psi(r)$ exists, and that

$$0 < \sin \Psi_R = -\frac{1}{R} \int_0^R \rho u(\rho) d\rho \leq 1.$$

We conclude also that if the solution curve does not cross the hyperbola $ru = -1$, then $\sin \Psi_R < 1$. The following assertion covers as well the case of solution curves crossing that hyperbola.

Iiii : Under the hypotheses of Iii, if in addition $u_0 \geq -2$, then $0 < \sin \Psi < 1$ in $0 < r \leq R$.

Proof: Consider the relation

$$(8) \quad \kappa_\ell + \kappa_m = \frac{\sin \Psi}{r} + (\sin \Psi)_r = -u,$$

the left side of which splits the mean curvature of the rotation surface defined by $u(r)$ into a sum of latitudinal (κ_ℓ) and meridional (κ_m) sectional curvatures. We note by Iii that $u(r)$ is increasing in $0 < r < R$; thus

$$(9) \quad \frac{\sin \Psi}{r} = -\frac{1}{r^2} \int_0^r \rho u(\rho) d\rho > -\frac{u(r)}{2}$$

in that interval. Integrating (8) with respect to u and noting that $(\sin \Psi)_r = -(\cos \Psi)_u$ yields, using (9),

$$\cos \Psi_R > 1 - \frac{1}{4} (u_0^2 - u_R^2)$$

which contains the assertion. We infer now from the general existence

theorem, applied at $r = R$, that the solution curve either can be continued upward until it crosses the r -axis, or else it tends asymptotically to this axis with increasing r . We may however exclude the latter possibility.

$$\text{Iiv : If } u(r) < 0 \text{ in } a \leq r < R < \infty, \text{ then } R < a \exp \left\{ - \frac{u_a}{a \sin \Psi_a} \right\}.$$

Proof: From (5) we find $r \sin \Psi > a \sin \Psi_a$ in $a \leq r < R$. By Iii, $\sin \Psi_a > 0$. Thus,

$$\frac{du}{dr} = \tan \Psi > \sin \Psi > \frac{a \sin \Psi_a}{r}$$

and the result follows on an integration.

We have thus established that if $u_0 \geq -2$ the solution curve is in its initial trajectory monotonically increasing and can be continued until it crosses the r -axis at a point $r = a_1$. To study the further trajectory, we observe that the curve can be continued at least locally across the axis as a solution of (5), and we compare its inclination at a given height h with the inclination of the initial branch at an equal negative height.

Iv : If the curve can be continued monotonically to a height h above the r -axis, then its inclination at this height is smaller than the inclination of the initial branch at the height $-h$, that is,

$$\left[\frac{du}{dr} \right]_h < \left[\frac{du}{dr} \right]_{-h}.$$

Proof: We integrate (8) with respect to u between the height $-h$ and h , obtaining

$$\cos \Psi \Big|_h - \cos \Psi \Big|_{-h} = \int_{-h}^h \frac{\sin \Psi}{r} du > 0.$$

Ivi : Under the conditions of Iiv, the curve is strictly convex downward when $u > 0$, and $u_{rr} < -u$.

Proof: From (8),

$$(\sin \psi)_r = \frac{u_{rr}}{(1 + u_r^2)^{3/2}} = -u - \frac{\sin \psi}{r} < -u.$$

From Iv and Ivi we find

Ivii : The curve can be continued to a maximum height $h_1 < |u_0|$ at a point $r = m_1 > a_1$, at which point $\sin \psi(m_1) = 0$.

We now proceed as above, comparing inclinations at corresponding heights until the curve crosses the r -axis a second time, then comparing inclinations as in Iv, and so on. We obtain the qualitative picture indicated in Theorem 1, of a curve oscillating about the r -axis with successively decreasing extrema (see Fig 1). We note also the additional information, yielded by the method:

Iviii : All inflections of the curve occur on (monotone) curve segments approaching the r -axis, in the sense of increasing s . At any two successive points α, β , at which $|u_\alpha| = |u_\beta|$, there holds

$$\left| \frac{du}{dr} \right|_\alpha > \left| \frac{du}{dr} \right|_\beta.$$

To prove the final statement of Theorem 1, we note by (7), Iii and Iviii that $|u_r(r; u_0)|$ tends uniformly to zero with u_0 ; thus the function $v(r; u_0) = u_0^{-1} u(r; u_0)$ tends uniformly to $J_0(r)$ as $u_0 \rightarrow 0$.

II Large $|u_0|$; initial arc

If $u_0 \ll 0$ the above reasoning on the behavior of the initial segment fails, and so do the results.

Theorem 2: If $(4) u_0 \leq -2\sqrt{2}$, there exists a value r_1 , beyond which $u(r)$ cannot be continued as a solution of (5). As $r \rightarrow r_1$, $\sin \psi \rightarrow 1$.

The proof could proceed by a direct study of the equation, as in section I. We obtain more precise results and also develop techniques that will be needed later if we proceed instead via an obvious comparison principle.

II i : Let $v^{(1)}(r)$, $v^{(2)}(r)$ be functions defined in $a \leq r \leq b$ and such that $(r \sin \psi^{(1)})_r \geq (r \sin \psi^{(2)})_r$. Suppose $\sin \psi^{(1)}(a) \geq \sin \psi^{(2)}(a)$. Then $\sin \psi^{(1)}(b) \geq \sin \psi^{(2)}(b)$, and equality holds if and only if $v^{(1)} = v^{(2)} + \text{const.}$ on $a \leq r \leq b$.

The interest in II i lies in the fact that $\frac{1}{r} (r \sin \psi)_r$ is exactly twice the mean curvature of the rotation surface defined by $u(r)$, and this circumstance facilitates the choice of comparison surfaces. In the present case we choose as initial comparison surface the sphere of constant mean curvature $-u_0/2$, with center at the point $(r, u) = (0, u_0 - 2/u_0)$. Thus, if $v(r)$ describes a vertical section of the sphere, there holds $u(0) = v(0)$, $u(r) < v(r)$ in the interval $0 < r \leq -\frac{2}{u_0}$ (see Fig 2). Using I ii, we find:

II ii : The solution $u(r)$ of (5, 6) can be continued at least until $r = -2/u_0$, and $\sin \psi(r) < -\frac{u_0 r}{2}$.

We need also:

II iii : A solution $u(r)$ of (5) admits no inflections in the region $ru < -1$.

Proof: From (8) follows $ru + \sin \psi = 0$ at any inflection.

Thus, ψ must continue to increase until either a vertical point is reached or the curve meets again the hyperbola $ru = -1$. Integrating (8) with respect to u and using II ii yields

$$1 - \cos \Psi > -\frac{1}{2} (u^2 - u_0 u).$$

From this we conclude that a vertical slope appears at a value

$$(10) \quad u_1 < \frac{u_0}{2} \left(1 + \sqrt{1 - 8/u_0^2} \right)$$

which completes the proof of Theorem 2.

We may use a similar procedure to estimate the value r_1 . We note that if $w(r)$ describes a vertical section of the sphere of constant mean curvature

$$(11) \quad \frac{1}{\beta} = -\frac{u_0}{4} \left(1 + \sqrt{1 - 8/u_0^2} \right)$$

with center at $(0, u_0 + \beta)$, then there holds $u(0) = w(0)$, and by II i $u'(r) > w'(r)$ on any interval $0 < r \leq R$ along which $\beta u \leq -2$. This condition is however satisfied at $u = u_1$ by (10), hence on the entire arc $u_0 < u \leq u_1$. We conclude $u(r) > w(r)$ until the first vertical occurs at $r = r_1 < \beta$.

We note that at $r = \beta$, where $w'(r) = \infty$, the circle $w(r)$ intersects the hyperbola $ru = -2$.

From II iii we conclude the initial solution curve is convex in the region $ru < -1$. This property holds in fact for the entire arc; on the segment of $u(r)$ joining the initial point to the point (r_c, u_c) on the hyperbola $ru = -1$ we obtain from (7, 8, I ii), using the comparison circle $v(r)$,

$$\kappa_m = (\sin \Psi)_r = -u - \frac{\sin \Psi}{r} > -v + \frac{u_0}{2} > -v(r_c) + \frac{u_0}{2} > 0.$$

The last relation holds whenever $u_0 \leq -\sqrt{2}$, which is the condition that $v(r)$ and the hyperbola $ru = -1$, $u < 0$ intersect. We conclude

also from I ii and the relation

$$(12) \quad \sin \Psi = -\frac{ru}{2} + \frac{1}{2r} \int_0^r \rho^2 u_\rho d\rho$$

that $ru > -2$ on the arc considered.

It turns out the sectional curvatures κ_l and κ_m are both monotone decreasing on the initial arc. We have

$$(13) \quad \frac{d}{dr} \kappa_l = \frac{d}{dr} \frac{\sin \Psi}{r} = \frac{2}{r^3} \int_0^r \rho u d\rho - \frac{u}{r} = \frac{1}{r} \left(-2 \frac{\sin \Psi}{r} - u \right) < 0$$

by (8, 12). Also, we have from (7, 8, I ii)

$$(14) \quad \begin{aligned} \frac{d}{dr} \kappa_m &= (\sin \Psi)_{rr} = -u_r + \frac{1}{r} \left(2 \frac{\sin \Psi}{r} + u \right) \\ &< -u_r + \frac{1}{r} (u - u_0) = -\frac{1}{r} \int_0^r \rho u_{\rho\rho} d\rho < 0 \end{aligned}$$

by the convexity of u .

At the initial point $(0, u_0)$ there holds $\kappa_l = \kappa_m = -u_0/2$. From (8, 12, I ii) follows for $r > 0$ on the initial arc

$$(15) \quad \kappa_m < -u/2 < \kappa_l$$

From (7, 8) we have also

$$(16) \quad \kappa_m = -u - \frac{\sin \Psi}{r} > -u + \frac{u_0}{2}.$$

The inequality (15) implies $\kappa_m < -u_0/2$, which is the meridional curvature of the comparison surface $v(r)$. Comparing the surface $u(r)$ with $v(r)$ at corresponding values of u and applying II ii now yields

$$(17) \quad u_1 > v\left(-\frac{2}{r_0}\right) = u_0 - \frac{2}{u_0}.$$

(see Fig. 2) .

We summarize the above results:

Theorem 3: Under the condition of Theorem 2, the initial arc of the solution curve, from (r_0, u_0) to (r_1, u_1) , is convex, with sectional curvatures κ_m, κ_1 decreasing and satisfying $\kappa_m < -u/2 < \kappa_1$ in $r_0 < r \leq r_1$. There holds ⁽⁴⁾

$$(18) \quad -\frac{2}{u_0} < r_1 < -\frac{u_0}{2} \left(1 - \sqrt{1 - \frac{8}{u_0^2}}\right)$$

$$u_0 - \frac{2}{u_0} < u_1 < u_0 - \frac{u_0}{2} \left(1 - \sqrt{1 - \frac{8}{u_0^2}}\right).$$

For $0 < r \leq -2/u_0$ the arc lies below the comparison circle $v(r)$ and has smaller curvature, and for $u_0 < u \leq u_1$ the arc lies above the comparison circle $w(r)$ and has larger curvature (see Fig. 2).

Further remark: The hypothesis $u_0 \leq -2\sqrt{2}$ of Theorem 2 could be sharpened by using the comparison surfaces $v(r)$ and $w(r)$ in (7) and iterating. A direct numerical integration of (7) yields [16] $u_0 \approx -2.5678$ as the value for which a vertical first appears. We find immediately:

II iv: Let u_{oc} be the largest value of u_0 for which a vertical point appears. If $u_0 = u_{oc}$ the vertical occurs at the second intersection of the solution curve with the hyperbola $ru = -1$, and is an inflection point for the solution curve (see Fig 3).

If $u_0 \leq -5$, the upper bounds in (18) can be expressed more simply, yielding

$$(19) \quad -\frac{2}{u_0} < r_1 < -\frac{2}{u_0} - \frac{5}{u_0^3}$$

$$u_0 - \frac{2}{u_0} < u_1 < u_0 - \frac{2}{u_0} - \frac{5}{u_0^3}$$

These bounds could also be improved by iteration, starting with the

comparison surfaces $v(r)$ and $w(r)$. We note for reference that the asymptotic series obtained in [16] by formal perturbation expansion yields, for the normalization used here,

$$(20) \quad \begin{aligned} r_1 &= -\frac{2}{u_0} - \frac{4}{3u_0^3} + O(u_0^{-5}) \\ u_1 &= u_0 - \frac{2}{u_0} - \frac{4 + 8 \ln 2}{3u_0^3} + O(u_0^{-5}) \end{aligned}$$

as $u_0 \rightarrow -\infty$.

III Very large $|u_0|$

If $u_0 \leq -2\sqrt{2}$ then $u(r)$ cannot be continued beyond r_1 as a solution of (2). The curve can, however, be continued as a solution of the parametric system (3) as long as r remains different from zero. We study now the behavior of this family of solutions in terms of the parameter u_0 , asymptotically as $u_0 \rightarrow -\infty$. We base the discussion principally on II i; to do so, we introduce as comparison functions the sections of rotation surfaces generated by the roulades of an ellipse. The following result is due to Delaunay [17]:

Let an ellipse of major axis $2a$ and distance $2c$ between focal points, roll rigidly on an axis without slipping. Let $\mathcal{C}$ be the curve swept out by one of the focal points. Then the surface generated by rotating $\mathcal{C}$ about the axis has constant mean curvature $H = (2a)^{-1}$.

We note that $\mathcal{C}$ is periodic with half-period τ satisfying $2a < \tau < \pi a$, and that each half-period can be represented in the interval $a - c \leq r \leq a + c$ by a single valued function $v(r)$ for which the equation

$$(21) \quad \frac{1}{r} (r \sin \psi)_r = 1/a$$

holds, and for which $\sin \psi = 1$ at the two end points (see Fig 4).

We proceed step by step :

The procedure of II shows that an infinite slope first appears at (r_1, u_1) , with bounds on (r_1, u_1) given by (18). The system (3) is non-singular at (r_1, u_1) , hence the curve can be continued beyond this point as a solution of (3, 4). From (16) we find at (r_1, u_1)

$$\kappa_m > -u_1 + \frac{u_0}{2} > \frac{u_0}{2} + \frac{2}{u_0} > 0$$

so the curve turns back toward the u -axis, and can be described again (locally) as a solution of (5). We compare it with a roulade $v^{(1)}(r)$ whose mean curvature is $-\frac{u_1}{2}$ and for which $a_1 + c_1 = r_1$ (see Fig 3). Since $v_r^{(1)}(r_1) = -\infty$, II i yields $u_r < v_r^{(1)}$, hence $u(r) > v^{(1)}(r)$ as long as the continuation of both u and $v^{(1)}$ as single valued functions is possible.

The curve $v^{(1)}(r)$ can be continued toward the u -axis only until the point $(a_1 - c_1, u_1 + \tau_1)$, with $a_1 - c_1 = -\frac{2}{u_1} - r_1 > 0$; at this point the slope is again infinite. It follows there is a value $r_2 > -\frac{2}{u_1} - r_1$ beyond which this branch of the solution curve cannot be continued as a single valued function.

From the geometrical interpretation of τ_1 as the half-circumference of an ellipse with major axis $2a_1 = -2/u_1$ and focal length $c_1 = r_1 - a_1$, one finds that for large $|u_0|$,

$$(22) \quad \tau_1 = -\frac{2}{u_1} + \alpha_1 \frac{\ln |u_1|}{|u_1|^3}, \quad \alpha_1 = -\frac{16}{3} + O\left(\frac{1}{\ln |u_1|}\right).$$

Let us estimate r_2 from above. To do so, we compare $u(r)$ with a roulade $\hat{v}_1(r)$, which is determined by the conditions

$$(23) \quad \hat{a}_1 = -\frac{1}{u_1 + \hat{\tau}_1}$$

$$\begin{aligned}
 \hat{a}_1 + \hat{c}_1 &= r_1 \\
 (23) \quad \hat{\tau}_1 &= \int_0^\pi \sqrt{a^2 - c^2 \cos^2 \theta} \, d\theta
 \end{aligned}$$

A formal estimate shows such a roulade exists if $u_1 < -2\sqrt{\pi}$.

The conditions (23) are chosen so that the roulade can be placed with its lower vertical point at (r_1, u_1) , (see Fig 5), and so that in that configuration its mean curvature will be exactly the one determined from the right side of (5) by the upper vertical. Applying II i we obtain

$$u_r > \hat{v}_r^{(1)}(r), \quad u(r) < \hat{v}^{(1)}(r) \quad \text{for all } r < r_1 \quad \text{for which } u(r) < u_1 + \hat{\tau}_1.$$

This condition clearly holds for r near r_1 ; since $\hat{v}^{(1)}(r) < u_1 + \hat{\tau}_1$, we conclude it holds on the entire interval $\hat{a}_1 - \hat{c}_1 < r < r_1$, thus

$$0 > v_r^{(1)}(r) > u_r(r) > \hat{v}_r^{(1)}(r) > -\infty$$

on this interval, and hence the solution can be continued to the left of r_1 , at least until the value

$$(24) \quad r_2 < -\frac{2}{u_1 + \hat{\tau}_1} - r_1 = \beta_2.$$

For large $|u_0|$ we find

$$(25) \quad \hat{\tau}_1 = -\frac{2}{u_1} + \hat{a}_1 \frac{\ln |u_1|}{|u_1|^3}$$

with

$$(26) \quad \hat{a}_1 = -\frac{40}{3} + O\left(\frac{1}{\ln |u_1|}\right).$$

Thus

$$(27) \quad r_2 < -\frac{2}{u_1} - \frac{\alpha_2}{u_1^3} - r_1$$

with

$$(28) \quad \alpha_2 = 4 + O(u_1^{-2} \ln |u_1|).$$

We now proceed, essentially, as in the proof of Theorem 2. We note

$$\sin \Psi > \sin \Psi^{(1)} = -\frac{ru_1}{2} + \frac{r_1}{r} \left(1 + \frac{r_1 u_1}{2}\right);$$

thus from (24-28) we find for $r < \beta_2$,

$$\frac{\sin \Psi}{r} > -\frac{3}{50} u_1^3 + O(u_1^{-5} \ln|u_1|).$$

We integrate (8) in u from $u(\beta_2)$; using that $\cos \Psi < 0$ until a vertical is reached, and that

$$\cos \Psi(\beta_2) > \cos \Psi^{(1)}(\beta_2) = -\frac{\sqrt{21}}{5} + O(u_1^{-2} \ln|u_1|)$$

we are led to a contradiction unless the curve becomes vertical before u has increased by a value $-16u_1^{-3}$. That is, a vertical must appear at a value

$$(29) \quad u_2 < u_1 + \hat{\tau}_1 - 16u_1^{-3}$$

The solution curve then turns back from the axis at (r_2, u_2) and initiates a further branch.

We summarize these results :

Theorem 4 : From (r_1, u_1) the solution curve continues backwards towards the u -axis until a second vertical is reached, at a point (r_2, u_2) with

$$(30) \quad -\frac{2}{u_1} - r_1 < r_2 < -\frac{2}{u_1 + \hat{\tau}_1} - r_1 = \beta_2$$

$$v^{(1)}(\beta_2) < u_2 < u_1 + \hat{\tau}_1 - 16u_1^{-3}.$$

In the interval $r_2 < r < r_1$ there holds $u_r < v_r^{(1)}$, $u > v^{(1)}$;

in the interval $\beta_2 < r < r_1$ there holds $u_r > \hat{v}_r^{(1)}$, $u < \hat{v}^{(1)}$.

We note in particular that the horizontal distance of the second vertical

from the axis exceeds that of the first vertical from the hyperbola $ru = -2$.

III i : There is exactly one inflection between (r_1, u_1) and (r_2, u_2) .

Proof: Clearly, at least one inflection appears. Using (8), we find

$$(ru + \sin \Psi)_r = \left(\frac{r}{\cos \Psi} - \frac{1}{r} \right) \sin \Psi < 0$$

on the arc. Hence there is at most one inflection.

We indicate briefly one further step in the procedure. We construct a roulade $v^{(2)}(r)$ passing through (r_2, u_2) , with major axis $2a_2 = -\frac{2}{u_2}$, and a second roulade $\hat{v}^{(2)}(r)$ with a property analogous to that introduced for $\hat{v}^{(1)}(r)$. Then there holds $\hat{v}_r^{(2)} < u_r < v_r^{(2)}$, $\hat{v}^{(2)} < u < v^{(2)}$ in the intervals for which the comparison makes sense, and (as before) still another point (r_3, u_3) is found such that $\sin \Psi(r_3) = 1$. The procedure can be continued as long as the values of $|u(r)|$ remain sufficiently large to justify the indicated steps.

We find easily:

III ii : The successive horizontal distances of the vertical points, from the axis and from the hyperbola, increase monotonically.

III iii : On each arc segment returning from the hyperbola to the axis there is exactly one inflection. The same statement holds on the remaining arc segments for sufficiently large $|u|$.

Theorem 5: In the initial region $u < 0$, the entire curve is bounded (strictly) between the u -axis and the hyperbola $ru = -2$ (see Fig 6). In this region, the curve can be represented by a single valued function $r = r(u)$, with $|r'(u)| < \infty$.

Proof: Since Theorem 4 and III i apply to any returning arc, we conclude the curve cannot contact the u -axis. The relation (9) shows

the curve does not meet the hyperbola on the initial arc starting from $(0, u_0)$. To show this property for any forward arc, we integrate (5) on such an arc from a vertical point (r_{2j}, u_{2j}) , obtaining

$$\begin{aligned} r \sin \psi - r_{2j} &= \frac{r_{2j}^2 u_{2j} - r^2 u}{2} + \frac{1}{2} \int_{r_{2j}}^r \rho^2 u' d\rho \\ &> -\frac{r_{2j}^2}{2} - \frac{r^2 u}{2} \end{aligned}$$

from which ^{follows} $ru > -2$ on this arc. The same inequality shows $\sin \psi > 0$ on this arc; an analogous integration establishes the same property on a returning arc.

IV Global behavior

The discussion thus far shows that the solution curve can be continued upward without self-intersections until it crosses the r -axis. For by I iii an outward branch must either achieve a vertical or cross that axis, and the comparison method of II yields readily that a returning branch has the same property. There are no horizontal points, by Theorem 5.

We show here that a returning branch cannot cross the r -axis. Precisely :

IV i : Let $r = a_1$ be the first point at which the solution curve meets the r -axis. Then $0 < u'(a_1) < \infty$.

Suppose $u'(a_1) < 0$, or equivalently, $\cos \psi_1 < 0$. The curve could then be continued backward into the negative u -plane ^{until} ~~to~~ a first vertical (r_α, u_α) (see Fig 7), at which, by Theorem 5,

$$(31) \quad r_\alpha u_\alpha > -2.$$

We integrate (8) with respect to u , from u_α to 0, obtaining

$$(32) \quad \int_{u_\alpha}^0 \frac{\sin \Psi}{r} du = \cos \Psi_1 + \frac{1}{2} u_\alpha^2.$$

To evaluate the left side of (32) we integrate (5) in r between r and r_α :

$$\begin{aligned} r_\alpha - r \sin \Psi &= - \int_r^{r_\alpha} \rho u d\rho < \frac{r^2 - r_\alpha^2}{2} u_\alpha \\ &< \frac{r^2 u_\alpha}{2} + r_\alpha \end{aligned}$$

by (31). Thus

$$(33) \quad \frac{\sin \alpha}{r} > - \frac{u_\alpha}{2}$$

on the entire arc. Placing (33) into (32) yields $\cos \Psi_1 > 0$, contradicting the assumption.

Now observe from (8) that at the crossing point a_1 , the meridional curvature is negative; thus, if $\cos \Psi_1 = 0$ there would again be a backward branch from a_1 into the negative u -plane, and we obtain a contradiction as above.

From IV i one sees immediately that the proof of Theorem 1 applies without change to the region $r \geq a_1$, in the sense that the solution curve continues from the point $(a_1, 0)$ as indicated in Fig. 1. We show now the curve does not intersect the initial branch in the region $u < 0$.

IVii: Let u_α, u_β be two successive points on the solution curve such that $r_\alpha = r_\beta$, with an intervening vertical at (r_γ, u_γ) . If $r_\gamma < r_\alpha$, then $\sin \Psi_\beta < \sin \Psi_\alpha$; if $r_\gamma > r_\alpha$, then $\sin \Psi_\beta > \sin \Psi_\alpha$.

Proof: Suppose $r_\gamma < r_\alpha$. From (5) we find

$$\begin{aligned} r_\beta \sin \Psi_\beta - r_\gamma &= - \int_{r_\gamma}^{r_\beta} \rho u d\rho \\ r_\alpha \sin \Psi_\alpha - r_\gamma &= - \int_{r_\gamma}^{r_\alpha} \rho u d\rho, \end{aligned}$$

thus since $r_\alpha = r_\beta$,

$$r_\alpha (\sin \Psi_\beta - \sin \Psi_\alpha) = \int_{r_\gamma}^{r_\alpha} \rho (u^- - u^+) d\rho < 0 ,$$

u^- and u^+ denoting values of u on the lower and upper branches.

The case $r_\gamma > r_\alpha$ follows similarly.

From IV ii follows $a < b$ in Fig. 8, and thus $h_1 < b$. But $h_j < h_1$, any $j > 1$, by I viii, hence $h_j < b$, all $j > 1$, and thus intersections are excluded.

Combining these results with Theorems 1 and 5 we obtain:

Theorem 6: The solution of the parametric system (3, 4) defined by the data u_0 can be continued indefinitely as a non-self-intersecting curve. It has the form indicated in Figs 1, 9, 10, 11.

V Maximum diameter

We define the diameter of a (symmetric) liquid drop as the largest diameter of all circular sections $u = u_j$, at which the bounding surface is vertical.

From Theorem 1, 5, 6 we see that each drop has a well defined diameter. It is less obvious that there is a universal upper bound for the diameters of all possible drops, independent of u_0 .

Theorem 7 : Let $\delta \sim 2.473$ be the unique positive root of the equation

$$(34) \quad r^3 - 3^{3/2} r - 3^{3/4} = 0.$$

Then 2δ exceeds the diameter of any solution of (3, 4).

We base the proof on a lemma, which also has an independent interest.

V i : Let $u(r)$ represent a solution curve passing through (a, u_a) with $-1 \leq au_a < 0$, and such that

$$(35) \quad a \sin \psi_a \geq a/2 .$$

Suppose $u(r) < 0$ in $a \leq r < R$. Then $\sin \psi > 0$ on this arc segment. If the curve meets the hyperbola $ru = -1$ in a point (c, u_c) with $a < c < R$, then $c < 3^{1/4}$, and $\sin \psi_c > 1/2$.

Proof: We integrate (5) between α and r , obtaining

$$(36) \quad r \sin \psi_r - \alpha \sin \psi_\alpha = \frac{1}{2} (\alpha^2 u_\alpha - r^2 u(r)) + \frac{1}{2} \int_\alpha^r \rho^2 u'(\rho) d\rho$$

from which, if $\alpha = a$,

$$(37) \quad r \sin \psi_r \geq -\frac{1}{2} r^2 u(r) + \frac{1}{2} \int_a^r \rho^2 u'(\rho) d\rho .$$

For r sufficiently near a , there holds $\sin \psi > 0$. Thus, if $\sin \psi$ were to vanish at any points interior to $a \leq r < R$, there would be a minimum $r = r_Y > a$ at which this occurs. But (37) would then imply

$$0 = r_Y \sin \psi_Y > \frac{1}{2} \int_a^{r_Y} \rho^2 u'(\rho) d\rho > 0,$$

a contradiction. Thus, $\sin \psi > 0$ on $a \leq r \leq c$, and hence $u'(\rho) > 0$ on this interval. Setting now $r = c$ in (37) yields

$$(38) \quad \sin \Psi_c > -\frac{1}{2} \quad cu(c) = \frac{1}{2}.$$

Finally, we note that at $r = c$ the inclination of the solution curve cannot exceed that of the hyperbola. Thus, $\sin \Psi_c < \frac{1}{\sqrt{1+c^4}}$, and $c^4 < 3$ follows from (38).

We proceed to prove Theorem 7. For any given u_0 , the maximum width is attained at a point (r_{2j+1}, u_{2j+1}) with $-1 \geq r_{2j+1} u_{2j+1} > -2$, $j \geq 0$ (see section III). At the preceding point (r_{2j}, u_{2j}) there holds either $r_{2j} = 0$ (if $j = 0$), or else $\sin \Psi_{2j} = 1$. In either event, (35) holds with $a = r_{2j}$. Also $-1 < r_{2j} u_{2j} < 0$, and thus the curve crosses the hyperbola $ru = -1$ at a point (c, u_c) , $r_{2j} < c < r_{2j+1}$. Setting $\alpha = c$, $r = r_{2j+1}$ in (36) and applying V i yields, using II iii,

$$(39) \quad r_{2j+1}^3 - 3^{3/2} r_{2j+1} - 3^{3/4} < 0.$$

The (single) positive solution of (34) exceeds any solution of (39). Since j is arbitrary, we conclude 2δ exceeds the diameter of any drop.

VI Convergence to the singular solution

The solutions discussed in this paper are apparently related to a singular solution $U(r)$ of (2), whose existence we have proved in [7]. The function $U(r)$ is defined in a deleted neighborhood of $r = 0$, and there holds asymptotically $U(r) \sim -\frac{1}{r}$, as $r \rightarrow 0$. We have conjectured that in any interval $0 < a \leq r \leq b < \infty$, the solutions of (3,4) admit a single valued representation $u(r; u_0)$ and converge uniformly to $U(r)$, as $u_0 \rightarrow \infty$. Figures 9, 10, 11 show the results of calculations supporting the conjecture. A preliminary (weak) form of the conjecture is proved in the complete, published version of this report [18].

VII ISOLATED CHARACTER OF GLOBAL SOLUTIONS

There is a strong numerical evidence to suggest that global solutions of (3) lying in the region between the envelope of the solutions $r(u;u_0)$ and the u axis, and without limit sets or self-intersections, are rare in the manifold of all solutions. We know of no such solutions, apart from those described in ^{this paper} $\wedge$ and the singular solution $U(r)$. In Fig. 12 are shown samples of the result of numerical integration of (3) through the initial point p determined by the intersection of $r(u;-8)$ with $U(r)$ and for varying initial angles α , measured counterclockwise from the arc of the curve $r(u;-8)$ emanating from p in the direction of increasing u .

We note the curves $r(u;u_0)$ can apparently be extended below the level $u = u_0$, if the isolated (singular) point of contact with the u -axis is admitted. The point appears to mark a transition in qualitative behavior; above it, the curve behaves like a Delaunay arc generated by an ellipse (section III). Below that point, the curve has the general appearance of a Delaunay arc generated by a hyperbola, with the characteristic double points of those arcs.

An analogous transition occurs on neighboring solutions without occurrence of singular points on the axis. In any event, if such singular points are admitted, the corresponding (extended) curves $r(u;u_0)$ are embedded naturally in a solution set, all of which develop double points for sufficiently negative u , with (we conjecture) the single exception of the solution $U(r)$.

We are indebted to Ivy Kuo for providing graphical capabilities to our computer program. Her contribution was an invaluable aid in developing the material of Section VII and for preparing Figure 12.

This work was supported in part by the Energy Research and Development Administration, by National Aeronautics and Space Administration, and by the National Science Foundation.

Footnotes

- (1) p1 For background information on the derivation of (1) see, e. g. [1, 2, 3].
- (2) p3 The remaining case can be realized physically, e. g., as the lower surface of a column of water in a glass capillary tube.
- (3) p4 We call attention however to a remarkable existence theorem due to Wente [9].
- (4) p5, 9, 12 This improves the result announced in [8].
- (5) p5 A stronger result of this type is given in [4].

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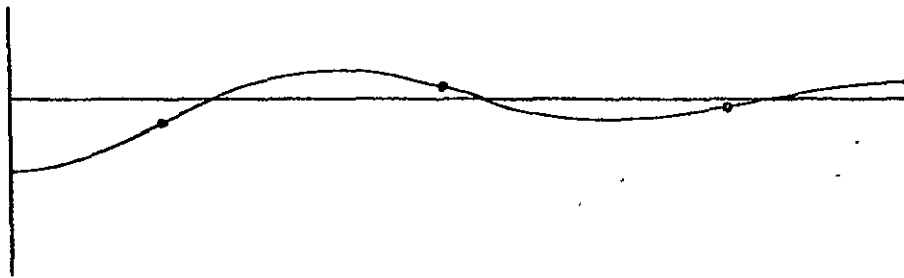


Figure 1

The case $u_0 \geq -2$; inflections

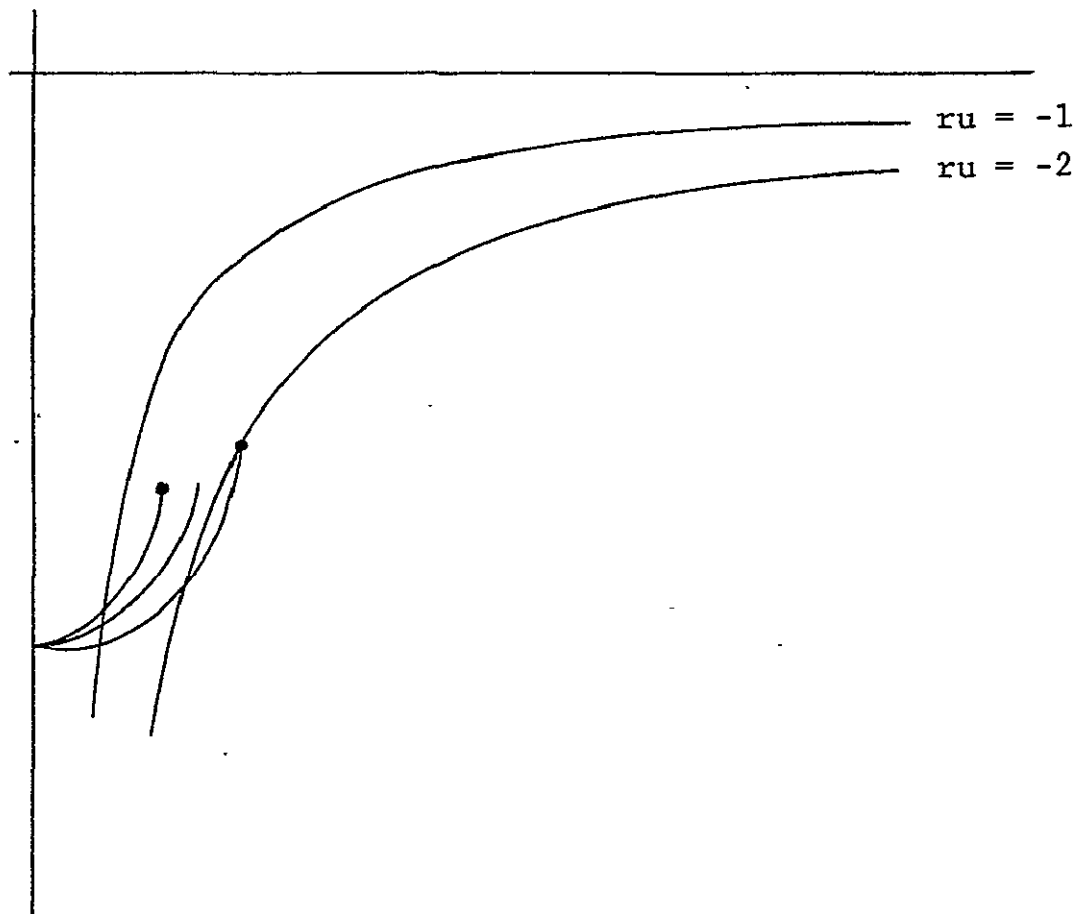


Figure 2

Initial comparison surfaces, $u_0 \leq -2\sqrt{2}$

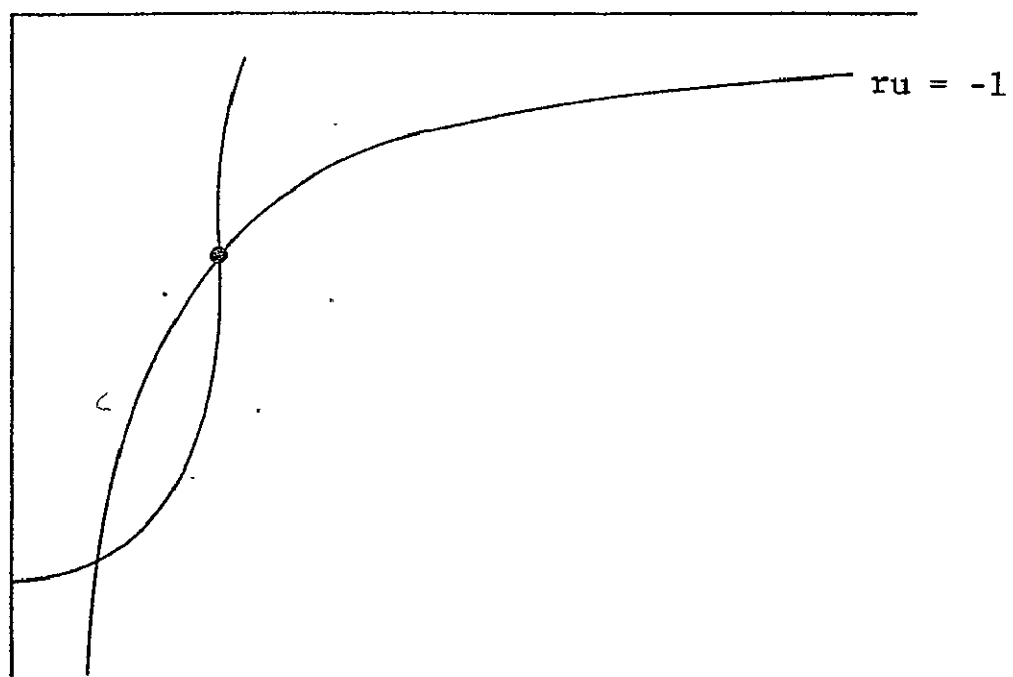


Figure 3

The case $u_0 = u_{oc}$

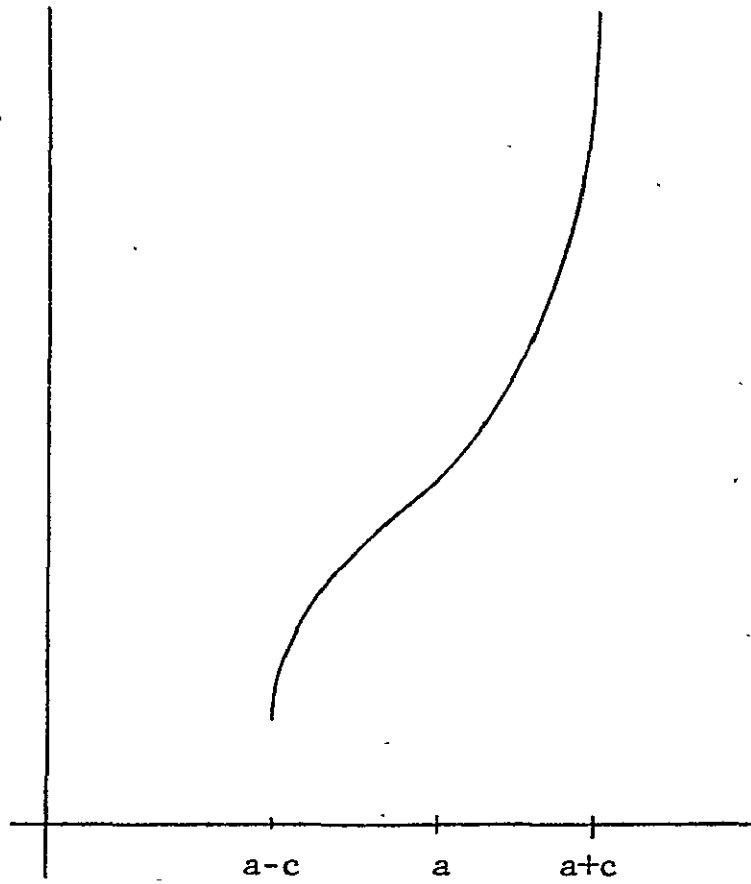


Figure 4

Delaunay surface

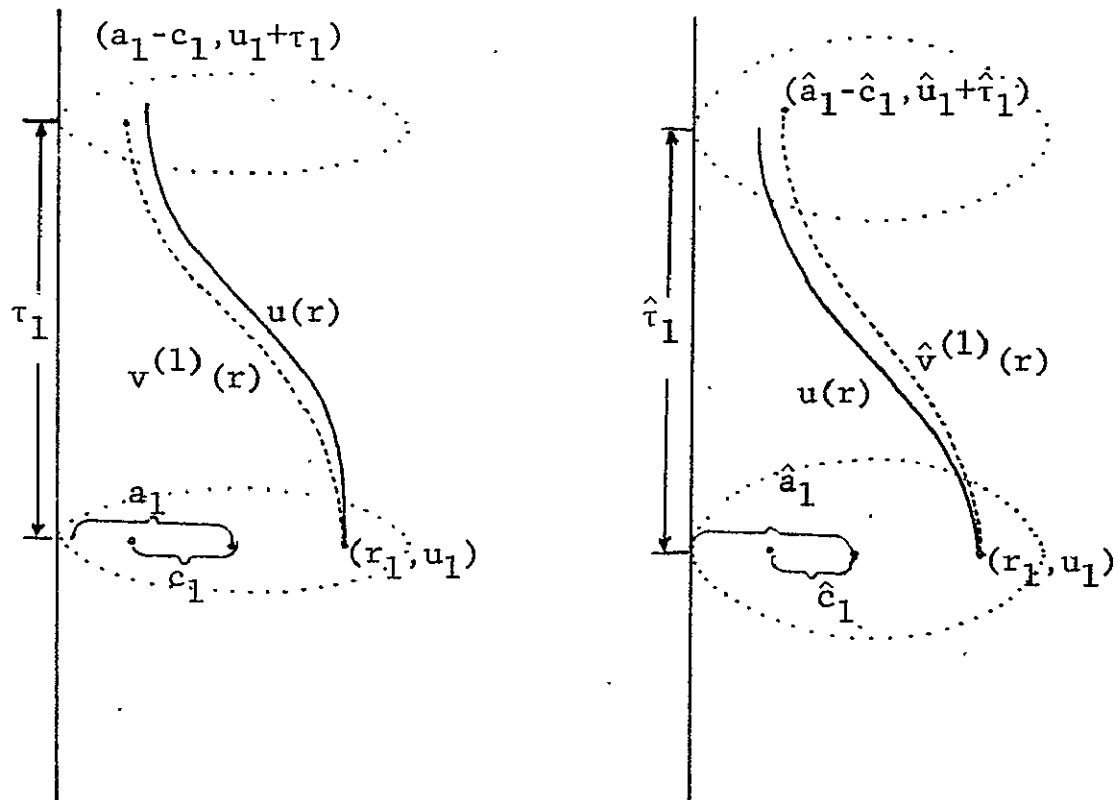


Figure 5

Comparison with roulades

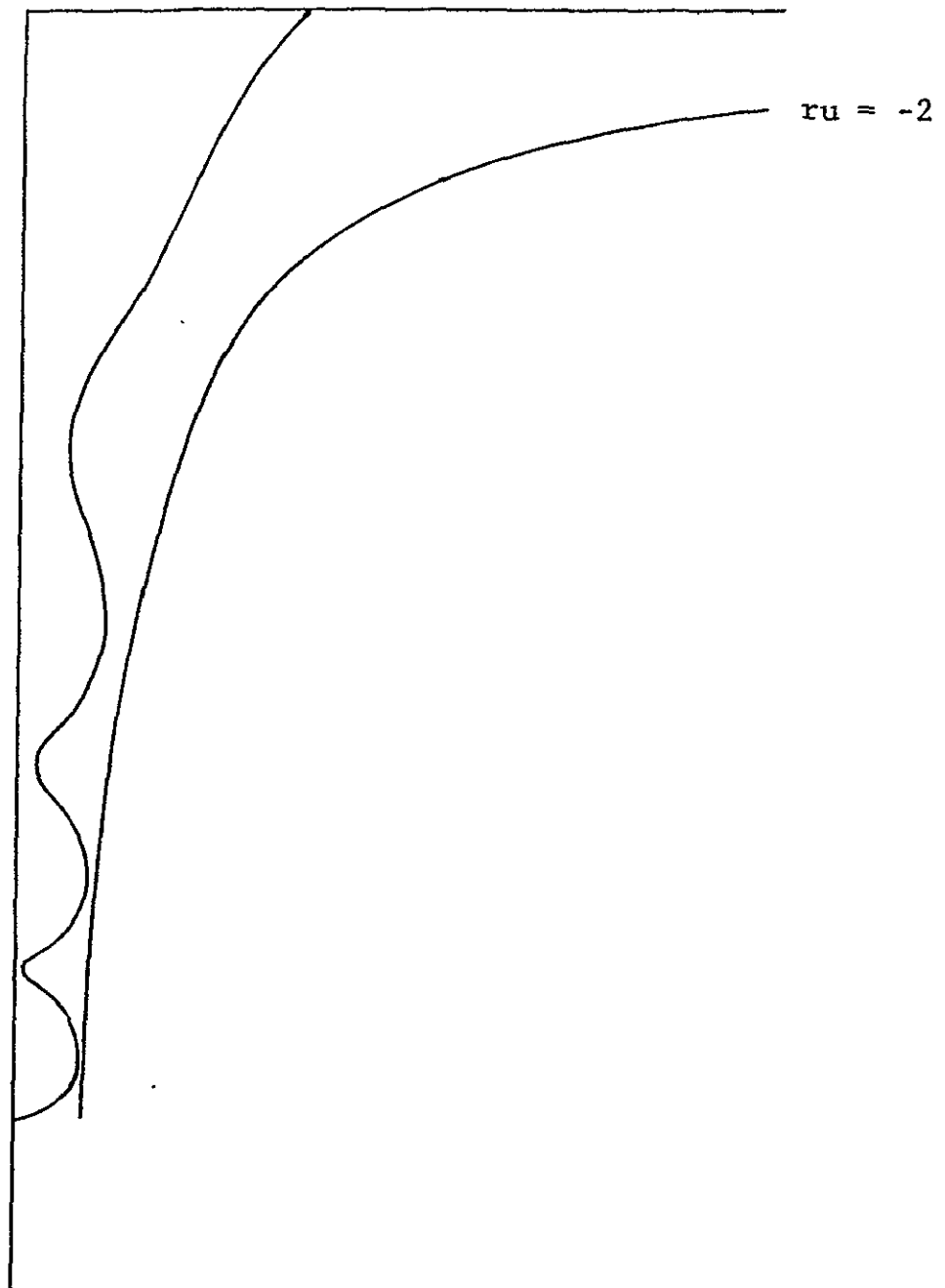


Figure 6

The initial region $u < 0$

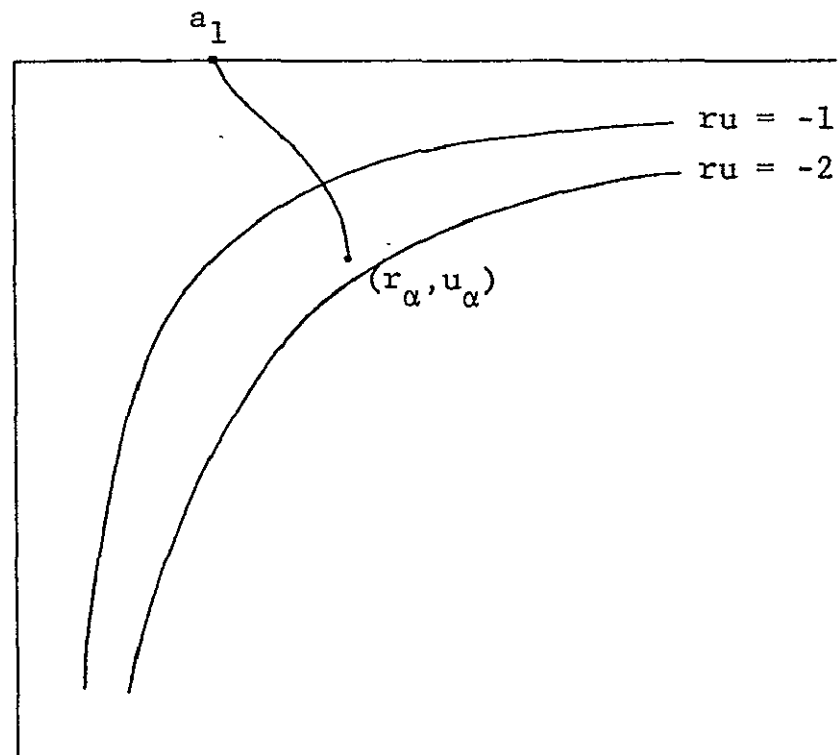


Figure 7

Proof of IV i

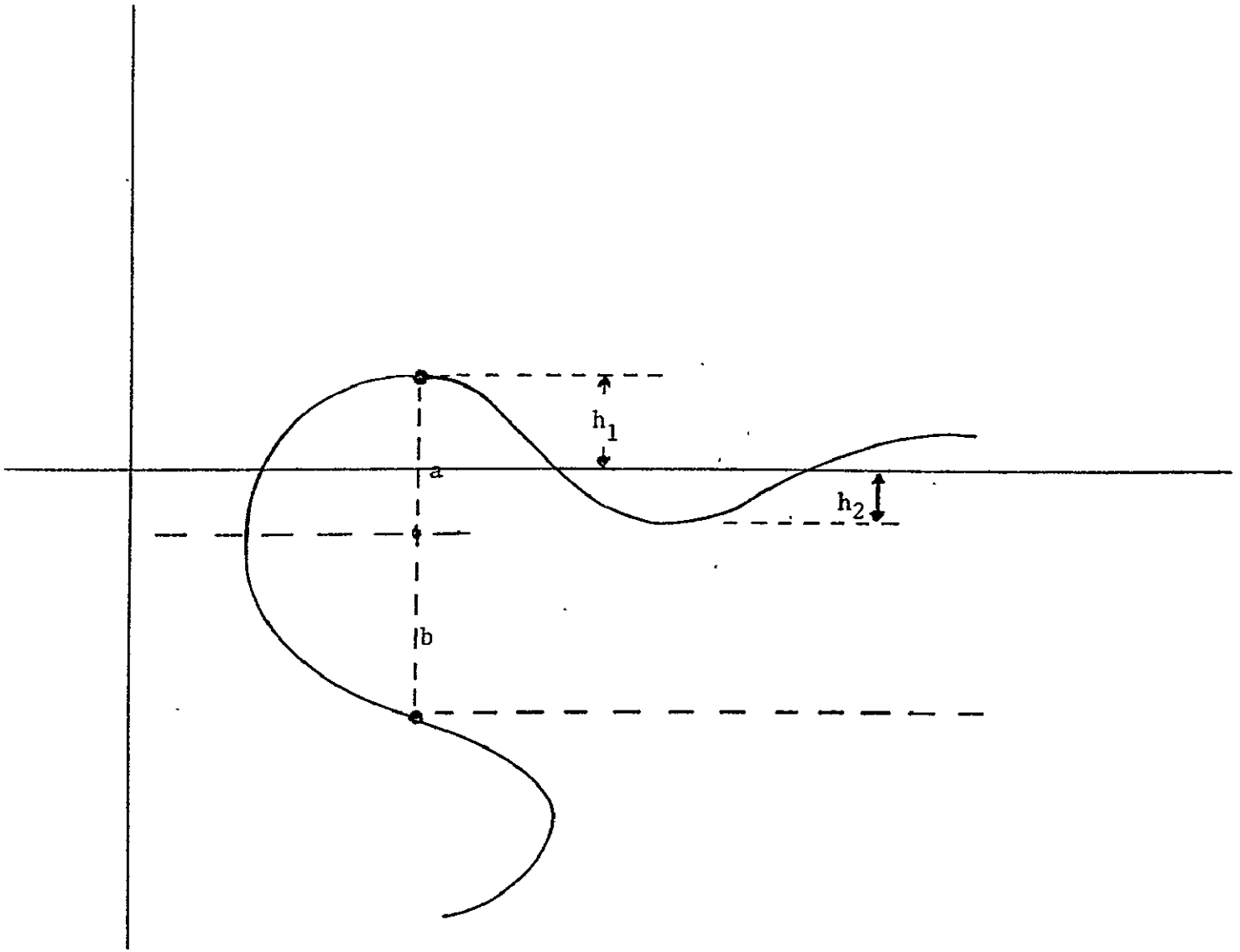
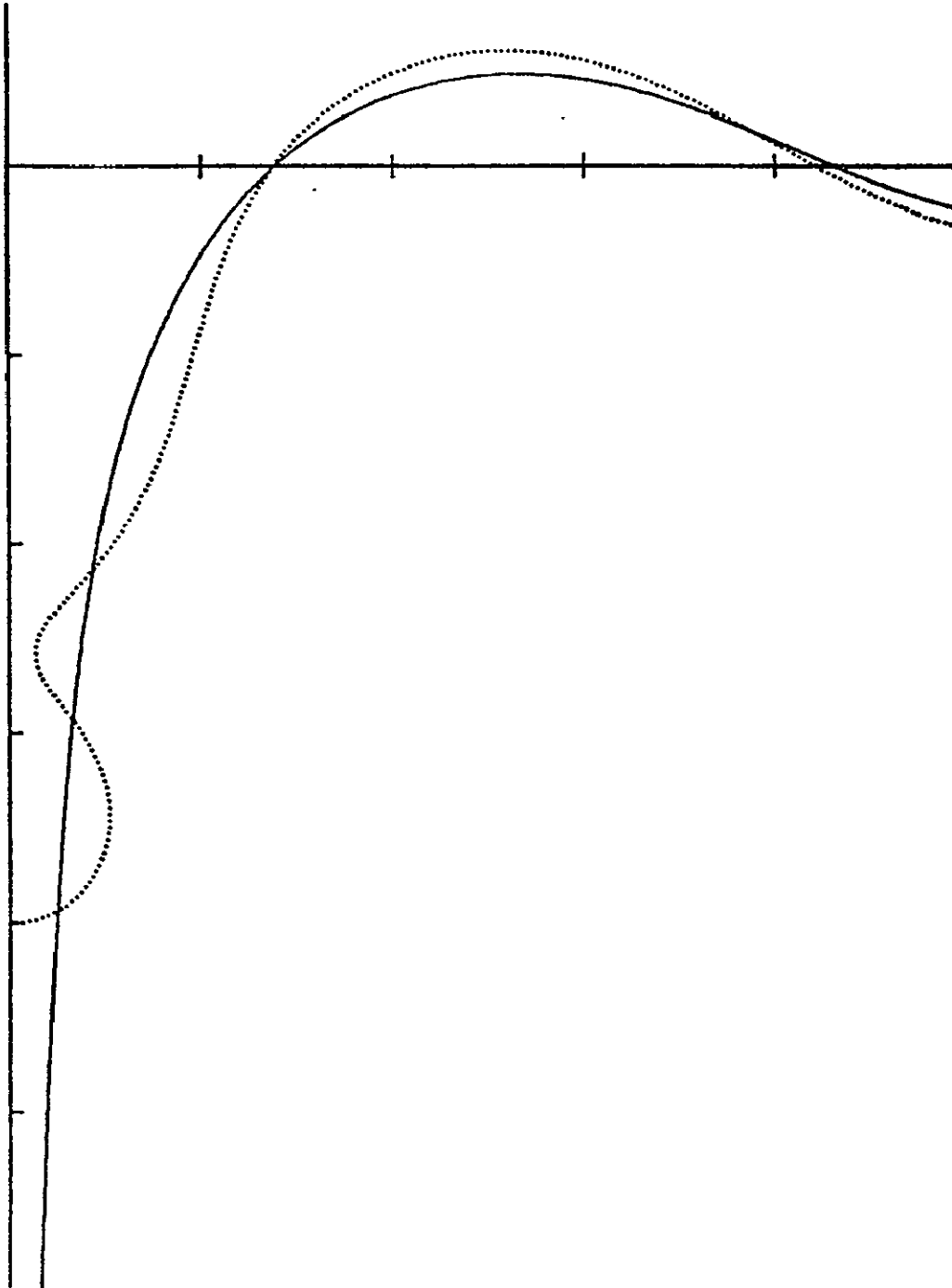


Figure 8. Proof of Theorem 6



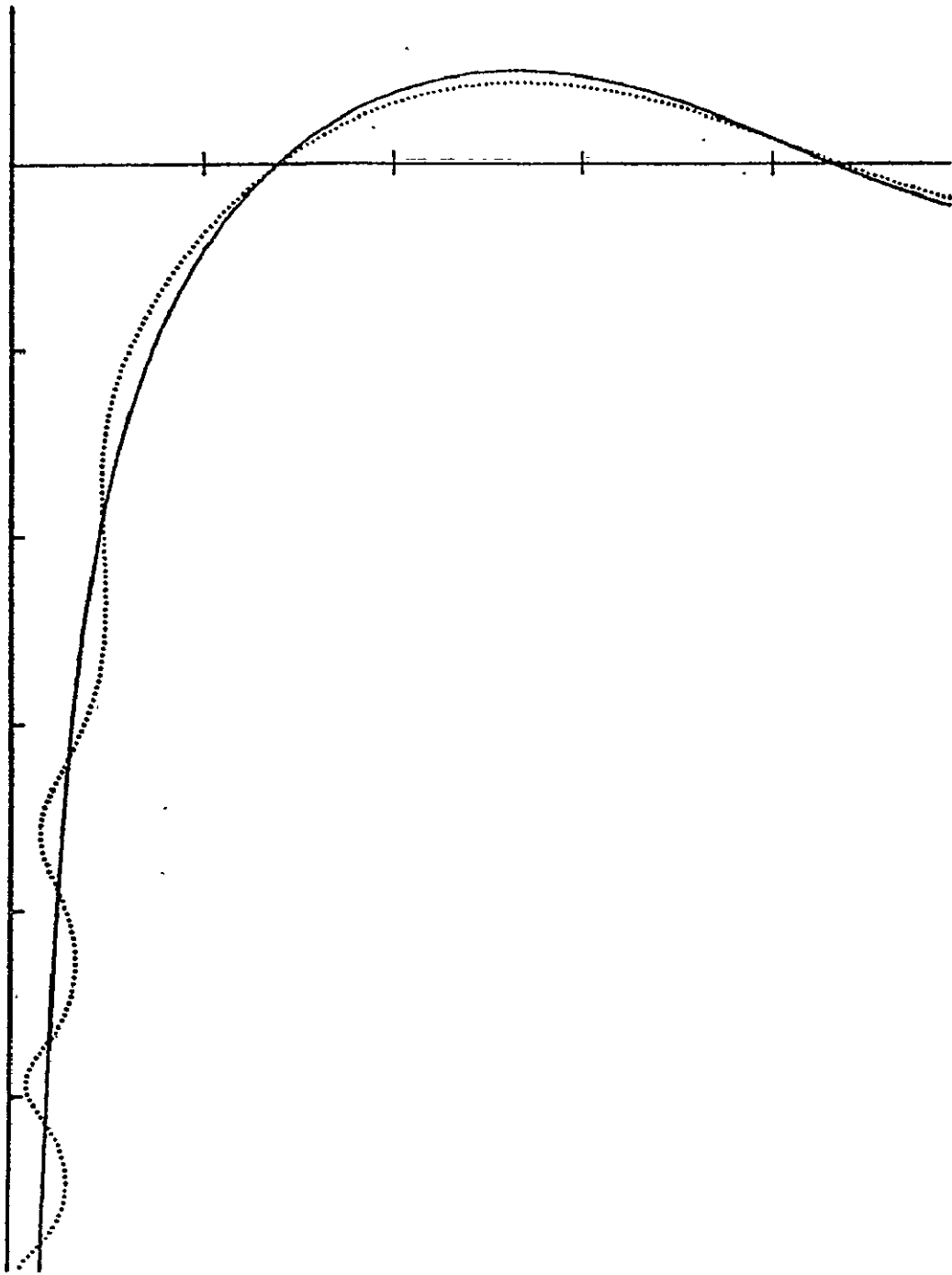


Figure 10

$u_0 = -8$; singular solution

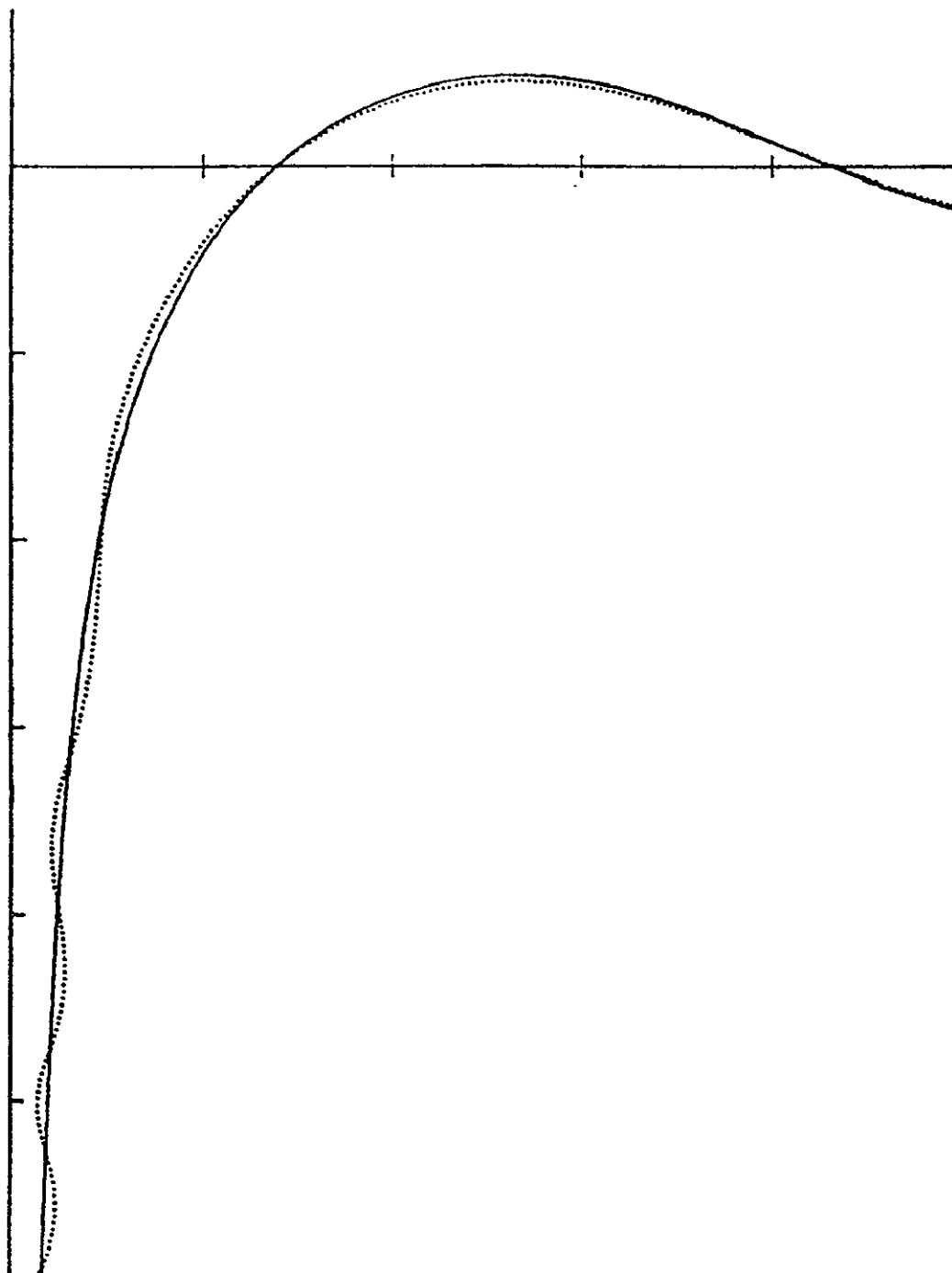
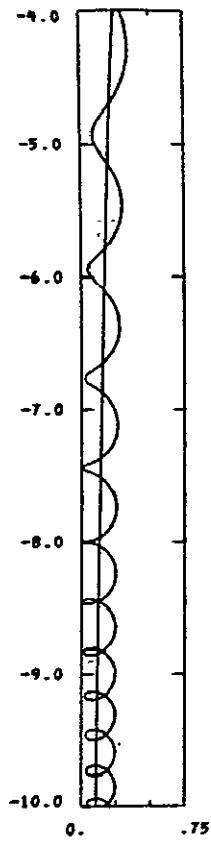
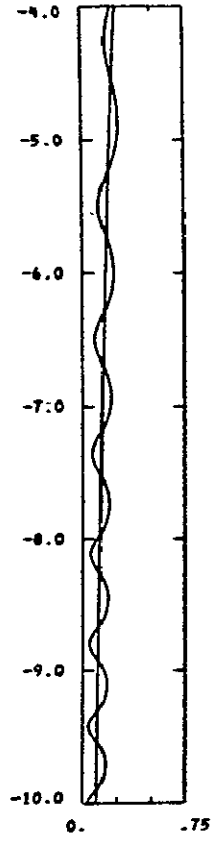
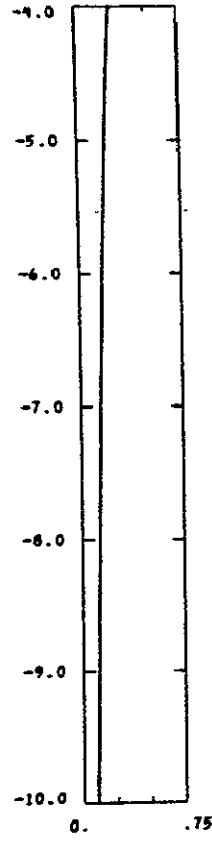
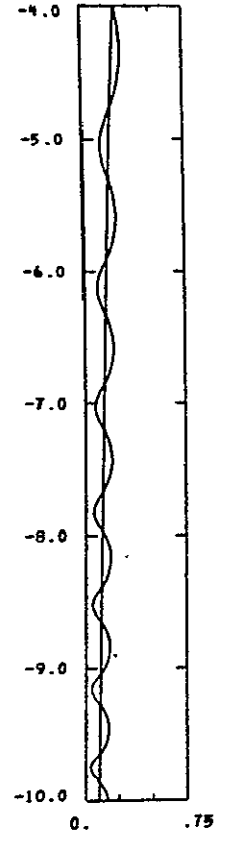
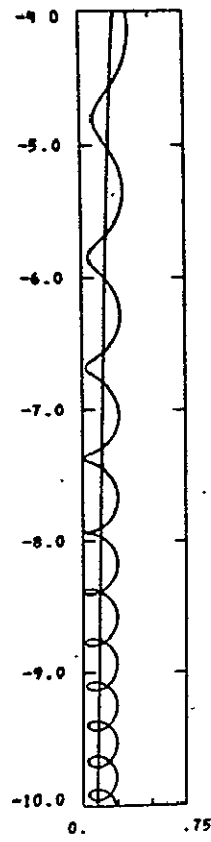
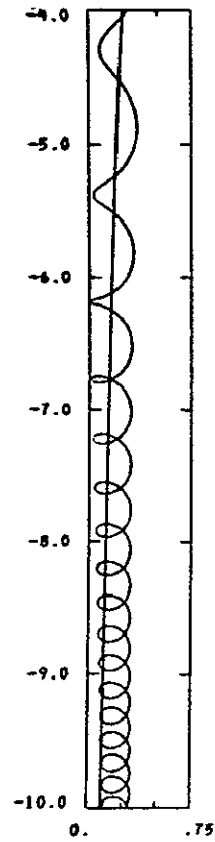
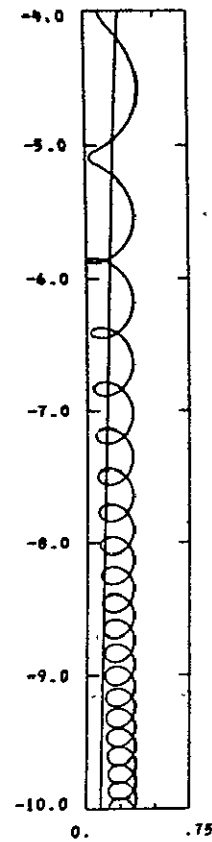
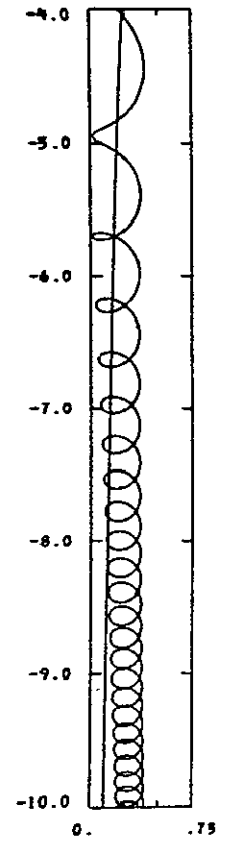
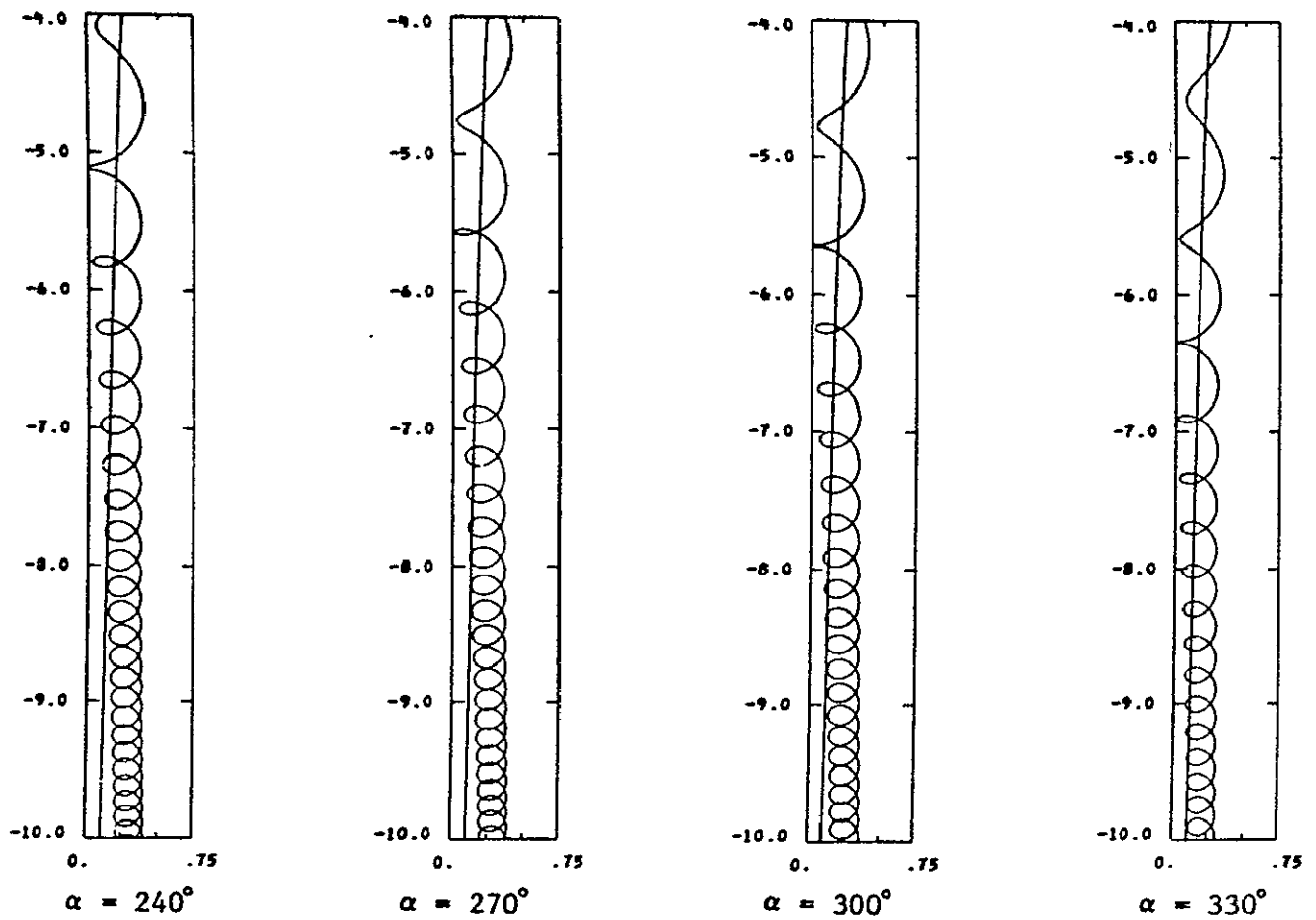


Figure 11

$u_0 = -16$; singular solution

 $\alpha = 0^\circ$  $\alpha = 30^\circ$  $\alpha = 60^\circ$  $\alpha = 90^\circ$  $\alpha = 120^\circ$  $\alpha = 150^\circ$  $\alpha = 180^\circ$  $\alpha = 210^\circ$



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Figure 12

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APPENDIX III

NUMERICAL SOLUTION OF THE CAPILLARY FREE
SURFACE EQUATION ON A SQUARE

by

Nai-Fu Chen and Paul Concus

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NUMERICAL SOLUTION OF THE CAPILLARY FREE
SURFACE EQUATION ON A SQUARE

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November 1977

ABSTRACT

Numerical methods are discussed for solving the partial differential equation describing the equilibrium free surface of a liquid in a vertical cylindrical container whose cross section has corners. Both the cases for which the free surface is bounded and for which it climbs infinitely high at a corner are considered. For the model problem of a container with square cross section comparative results of numerical experiments are given for a nonlinear relaxation method, for a conjugate gradient method, and for several techniques for handling the corner singularity utilizing the known asymptotic form of the solution. Representative solution surfaces are depicted graphically.

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1. Introduction

In this paper, we discuss algorithms for solving numerically the nonlinear partial differential equation describing the equilibrium free surface of a liquid under surface and gravitational forces. We are interested particularly in the case of a liquid partly filling a vertical cylinder, the cross section of which has corners. We assume that the surface height $u(x,y)$ is a single-valued smooth function of x and y , that there is sufficient liquid to cover the cylinder base entirely, and that the gravitational field is uniform and directed vertically downward. Then the function $u(x,y)$ satisfies

$$\frac{\partial}{\partial x} \left(\frac{1}{W} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{1}{W} \frac{\partial u}{\partial y} \right) = Bu + 2H, \quad (1)$$

$$W = [1 + (\partial u / \partial x)^2 + (\partial u / \partial y)^2]^{\frac{1}{2}}$$

where $B = \rho_0 g / \sigma$ with ρ_0 the difference in densities between the gas and liquid phases, g the gravitational acceleration (positive when directed downward), and σ the gas-liquid interfacial surface tension. The quantity $2H$ is a constant determined, in general, by the shape of the cylinder cross section, the volume of liquid, and the boundary condition between the liquid surface and the cylinder wall. The mean curvature of the surface is H at points where $u=0$. We consider only the case $B > 0$. The parameter B is the (dimensionless) Bond number, if (1) is considered to have been made nondimensional with respect to a characteristic length of unity.

Let the prescribed angle of contact between the liquid free-surface and the cylinder wall, measured interior to the liquid, be denoted by

the constant γ . This condition can be written as

$$\frac{1}{W} \frac{\partial u}{\partial n} = \cos \gamma \quad \text{at the cylinder wall,} \quad (2)$$

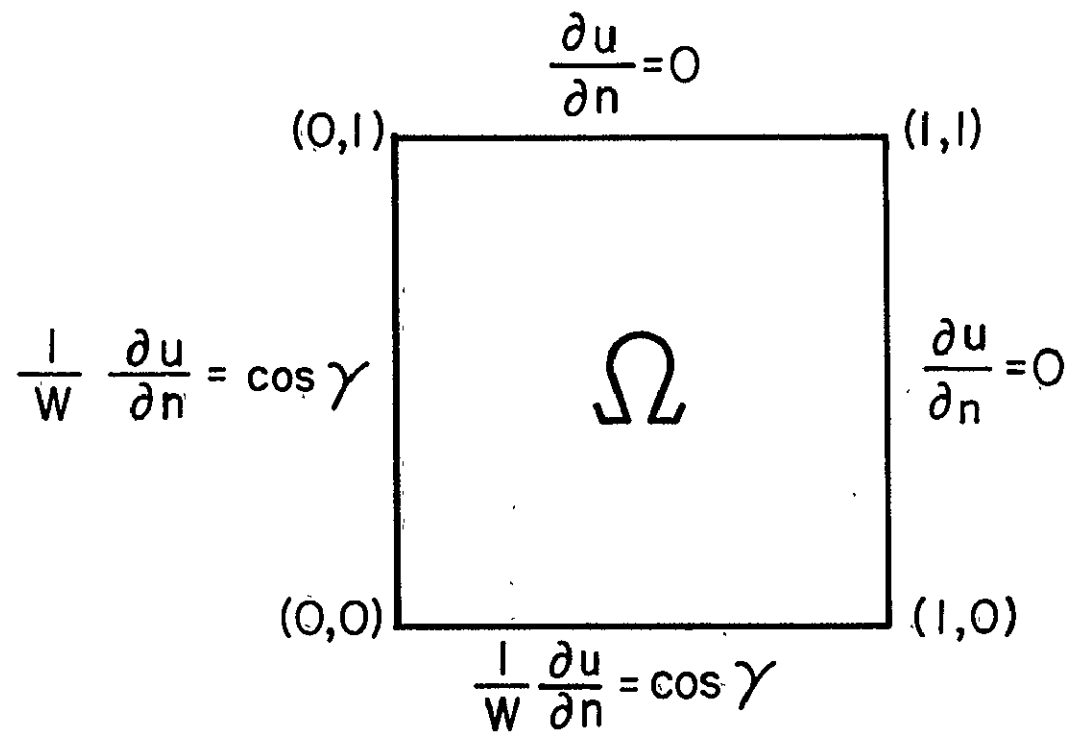
where $\partial u / \partial n$ is the derivative of u with respect to the outward normal. We consider here only the case of wetting liquids, $0 \leq \gamma < \pi/2$. (The complementary case of non-wetting liquids can be derived from it directly by means of a simple transformation.)

The value of the contact angle plays a crucial role in determining the qualitative nature of the solution when the domain under investigation contains corners. Let the interior angle of a corner be 2α ; it is proved in [6,7] that the solution at the vertex of the corner is bounded if and only if $\alpha + \gamma \geq \pi/2$. For the case $\alpha + \gamma < \pi/2$ set $\kappa = \sin \alpha \sec \gamma$ and introduce polar coordinates ρ, θ with origin at the vertex and θ measured from the interior angle bisector. Consider the function

$$v(x,y;\gamma) = \left[\cos \theta - (\kappa^2 - \sin^2 \theta)^{1/2} \right] / (\kappa B \rho), \quad (3)$$

for $-\alpha \leq \theta \leq \alpha$, $\rho > 0$. It is shown in [5] that there exists a constant C such that the solution $u(x,y)$ satisfies $|u(x,y) - v(x,y)| < C$ for sufficiently small ρ . Because of the differing qualitative natures of the bounded and unbounded solutions, we treat these two cases separately.

We take the 2×2 square as the domain for our model problem. Because of the symmetry, we consider only the equivalent problem on a 1×1 square with boundary conditions as shown in Figure 1. We place a uniform square grid of width $h=1/N$ on the domain and discretize (1) in a manner similar to that used in [3] for the minimal surface equation ($B=H=0$), which is related to the general procedure in [11] for linear elliptic equations.



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Fig. 1

The domain Ω for the model problem.

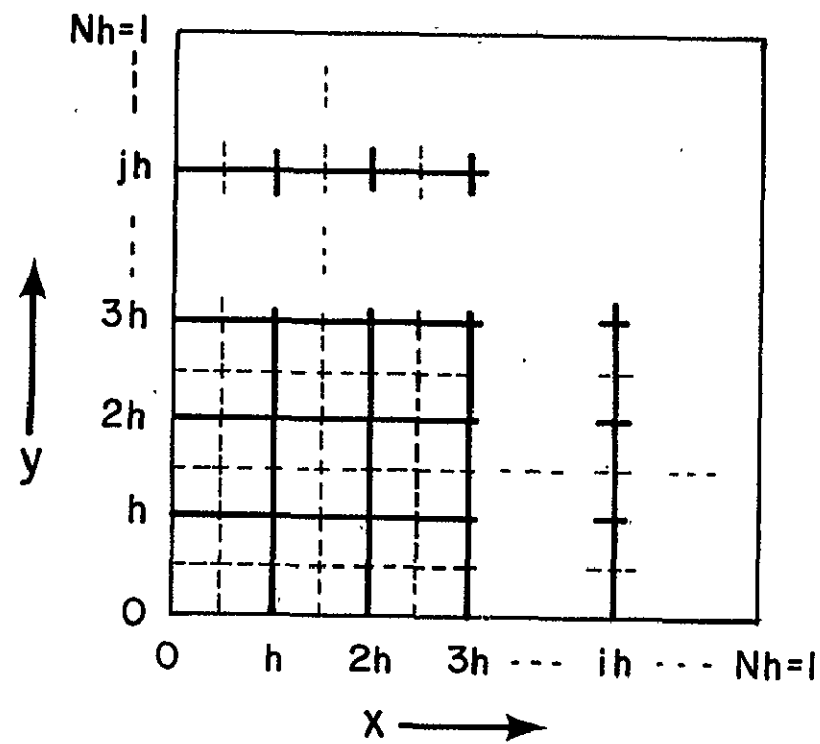
We write the integral form of (1), as obtained by use of Green's theorem, over a sub-domain D of Ω , which yields

$$\int_{\partial D} \frac{1}{W} (\nabla \mathbf{u} \cdot \underline{n}) d\ell = \iint_D (Bu + 2H) dA, \quad (4)$$

where $\underline{n}$ is the outward unit normal and ∂D is the boundary of D .

Then we place on Ω an auxiliary mesh (the dotted lines bisecting the original mesh lines in Fig. 2). We denote an $h \times h$ square bounded by the original grid lines as a cell, and we denote a rectangle bounded by auxiliary grid lines, and possibly $\partial\Omega$, as an auxiliary cell. By imposing (4) on each of the auxiliary cells and using the midpoint rule for integration, we obtain a set of (nonlinear) algebraic equations. The equation corresponding to a typical interior point $u(x,y)=u(ih,jh)=U_{i,j}$ is given by

$$\begin{aligned} f_{i,j} = & W_{i,j}^{-1} \left(2U_{i,j} - U_{i-1,j} - U_{i,j-1} \right) \\ & + W_{i+1,j}^{-1} \left(2U_{i,j} - U_{i+1,j} - U_{i,j-1} \right) \\ & + W_{i,j+1}^{-1} \left(2U_{i,j} - U_{i-1,j} - U_{i,j+1} \right) \\ & + W_{i+1,j+1}^{-1} \left(2U_{i,j} - U_{i+1,j} - U_{i,j+1} \right) \\ & + 2h^2 \left(BU_{i,j} + 2H \right) = 0, \end{aligned} \quad (5)$$



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Fig. 2

The domain with the original grid and the auxiliary grid.

where
$$W_{\bar{i}, \bar{j}} = \left[1 + \frac{1}{2} \left(\delta_{\bar{i}, \bar{j}}^2 + \delta_{\bar{i}, \bar{j}-1}^2 + \eta_{\bar{i}, \bar{j}}^2 + \eta_{\bar{i}-1, \bar{j}}^2 \right) \right]^{1/2},$$

with
$$\delta_{\bar{i}, \bar{j}} = (U_{\bar{i}, \bar{j}} - U_{\bar{i}-1, \bar{j}})/h \text{ and } \eta_{\bar{i}, \bar{j}} = (U_{\bar{i}, \bar{j}} - U_{\bar{i}, \bar{j}-1})/h.$$

Notice that the integration of (4) is performed over each auxiliary cell, and we use the approximation $\iint_D (Bu + 2H) dA \approx (BU_{\bar{i}, \bar{j}} + 2H) \cdot (\text{area of } D)$. Note also that in the discrete equations we take W to be constant over each cell $= (W_{\bar{i}, \bar{j}} \text{ for the cell centered at } (i-1/2, j-1/2))$. For a boundary segment $\partial\Omega_s$ of $\partial\Omega$ we have

$$\int_{\partial\Omega_s} \frac{\nabla u \cdot \underline{n}}{W} d\ell = \begin{cases} \cos\gamma \cdot (\text{length of } \partial\Omega_s), & \text{if } W^{-1} \partial U / \partial n = \cos\gamma \\ 0 & , \text{ if } \partial u / \partial n = 0. \end{cases}$$

In the following sections, we shall discuss and compare different methods for solving the discrete equations, for the bounded and unbounded cases.

2. The Bounded Case

In this section, we investigate two methods for obtaining the solution of the discrete form of (1), (2) for the bounded case $(\alpha + \gamma \geq \pi/2)$, which for the square $(\alpha = \pi/4)$ is the case $\gamma \geq \pi/4$.

2.1. Block SOR-Newton

Here, we use the nonlinear block successive overrelaxation method investigated in [4] for solving the minimal surface equation and described in [10] as the one-step block successive overrelaxation-Newton (BSOR-Newton) method. A block SOR iteration, corresponding to a row of mesh points, is performed using a single Newton iteration to solve approximately the resulting system of nonlinear equations. We thus "solve" for one row of mesh points (see figure 2) at a time by considering the function values in that row $U_{i,j}$, $0 \leq i \leq N$, to be the only unknowns and using the latest values for all other $U_{i,j}$. If we denote by U_J , f_J the vectors $U_J = (U_{0,j}, U_{1,j}, \dots, U_{N,j})$, $f_J = (f_{0,j}, f_{1,j}, \dots, f_{N,j})$, and by J_{JJ} the matrix $J_{JJ} = (\partial f_{i,j} / \partial U_{k,j}), i, k = 0, 1, \dots, N$ evaluated at the current value of $U_{i,j}$, we have the iteration

$$J_{JJ}\chi = f_J$$

$$U_J^{(\ell+1)} = U_J^{(\ell)} - \omega\chi$$

where ω is the relaxation parameter. J_{JJ} is symmetric, positive-definite, and tridiagonal, thus the solution of $J_{JJ}\chi = f_J$ can be obtained efficiently using Gauss elimination without pivoting, or Cholesky decomposition.

By differentiating (5), we obtain explicit expressions for the partial derivatives at a general interior point:

$$\begin{aligned} \frac{\partial f_{i,j}}{\partial U_{i,j}} = & 2 \left(W_{i,j}^{-1} + W_{i+1,j}^{-1} + W_{i,j+1}^{-1} + W_{i+1,j+1}^{-1} + Bh^2 \right) \\ & + \dot{W}_{i,j}^{-1} \left(\delta_{i,j} + \eta_{i,j} \right)^2 + \dot{W}_{i+1,j}^{-1} \left(-\delta_{i+1,j} + \eta_{i,j} \right)^2 \\ & + \dot{W}_{i,j+1}^{-1} \left(\delta_{i,j} - \eta_{i,j+1} \right)^2 + \dot{W}_{i+1,j+1}^{-1} \left(-\delta_{i+1,j} + \eta_{i,j+1} \right)^2, \end{aligned}$$

$$\begin{aligned} \frac{\partial f_{i,j}}{\partial U_{i-1,j}} = & -W_{i,j}^{-1} - W_{i,j+1}^{-1} \\ & + \dot{W}_{i,j}^{-1} \left(\delta_{i,j} + \eta_{i,j} \right) \left(-\delta_{i,j} + \eta_{i-1,j} \right) \\ & + \dot{W}_{i,j+1}^{-1} \left(\delta_{i,j} - \eta_{i,j+1} \right) \left(-\delta_{i,j} - \eta_{i-1,j+1} \right), \end{aligned}$$

and, by symmetry, $\partial f_{i,j} / \partial U_{i+1,j} = \partial f_{i+1,j} / \partial U_{i,j}$. Here

$$\dot{W}_{i,j}^{-1} = \left[d(W^{-1}) / d|\nabla U|^2 \right]_{i,j} = -\frac{1}{2} (1 + U_x^2 + U_y^2)^{-3/2} \text{ evaluated for cell } i,j$$

(see [3][4]).

After each iteration we adjust the value of H , using (4) integrated over Ω . The left hand side yields $2 \cos \gamma$ and the right hand side, after discretization, $B\bar{U} + 2H$, where $\bar{U}$ is the area-weighted average of $U_{i,j}$. The adjustment of H , which enhances the rate of convergence, corresponds to an adjustment of the volume of liquid. A final adjustment can be made, if desired, after the solution has been obtained, by moving the solution vertically to correspond to a particular liquid volume.

The convergence rate of the BSOR-Newton method depends critically on the choice of the relaxation parameter ω . Table 1 compares the number of iterations required to decrease the residual $\|f\|_2$ from its initial value of approximately 0.5 to $\leq 10^{-6}$, with zero initial approximation, $\gamma = \pi/3$, $B=100$, and $h=1/40$.

As obtained from our experiments, the estimated asymptotically optimal value of ω for the above case is 1.58. In general, it may be necessary to use a value of ω smaller than the optimal one to ensure convergence for a given initial approximation (see Tables 1 and 2). The number of iterations required for convergence can be reduced in these cases by adjusting ω towards the asymptotically optimal value as the iteration proceeds, once the approximation to U becomes sufficiently good to permit doing so. Each complete SOR sweep (for the 41×41 grid) takes approximately 0.055 sec. on the CDC 7600 computer (using a FORTRAN program with the FTN4 compiler, OPT = 2).

Table 1. Number of iterations required for convergence for
 $\gamma = \pi/3$, $B=100$, $U^{(0)} \equiv 0$ and $h=1/40$.

number of iterations	ω	1.2	1.3	1.4	1.5	1.6	1.7	1.8
		>100	90	72	56	44	divergence	divergence

We have tried an initial approximation of zero for this problem, and the one of U equal to the portion of the lower hemisphere satisfying (1) and (2) for $B=0$ and $\gamma = \pi/4$. For these two initial approximations, the number of iterations required for convergence was essentially the same, when convergence occurred. Changing the contact angle did not affect the convergence rate substantially either, except that convergence was more rapid when γ was close to $\pi/2$.

Table 2. Number of iterations for convergence for $B=100$, $h=1/40$, and $\Pi(o) = 0$.

$\gamma \backslash \omega$	1.4	1.5	1.6
$\pi/4$	72	56	divergence
$\pi/3$	72	56	44

The size of B substantially affects the number of iterations required for convergence. The smaller B is, the larger the number of iterations required to reduce the relative error below the desired tolerance, and the stronger the dependence on ω . Table 3 compares behavior for a few values of ω for the problem $\gamma = \pi/4$, $B=1$ with zero initial approximation, and $\|f^{(k)}\|_2 \leq 10^{-6}$.

Table 3. Number of iterations for convergence for $B=1$, $\gamma = \pi/4$, $h=1/40$,

$$\underline{U^{(0)} \equiv 0.}$$

ω	1.5	1.8*	1.84*
number of iterations	>200	191	123

* ω was set equal to 1.5 initially to prevent divergence and was later increased progressively to the indicated value.

The slower convergence for smaller B should be expected, since for the boundary conditions (2), or those in Fig. 1, the problem becomes singular when $B=0$.

Judging from the experimental results, if either we have a priori knowledge of an optimal value for ω or if a scheme for improving ω is incorporated into the program, this overrelaxation method is quite efficient for larger values of B . We should add here that this method works also for the case $B=0$, for which a closed-form solution is known. We discuss further experimental results for the behavior of the BSOR-Newton method in Sec. 2.3, where a comparison is made with results for the method discussed in the following section.

2.2. Hybrid conjugate gradient method

In this section, the conjugate gradient method is combined with a fast Helmholtz solver to obtain iteratively the solution to the discrete

form of (1) and (2). This method proceeds as follows (see [8]):

(i) Given an initial approximation $U^{(0)}$ ($U^{(0)}$ is a vector of length $(N+1)^2$). Arbitrarily define $p^{(-1)}$. For $k = 0, 1, 2, \dots$

(ii) Compute

$$f^{(k)} = f_{ij}(U^{(k)})$$

and solve $Mz^{(k)} = -f^{(k)}$.

(iii) Compute the search direction

$$p^{(k)} = z^{(k)} + \beta_k p^{(k-1)},$$

$$\text{where } \beta_k = \frac{(f^{(k+1)}, z^{(k+1)})}{(f^{(k)}, z^{(k)})} \quad k \neq 0, m, 2m, 3m, \dots$$

$$\beta_0 = \beta_m = \beta_{2m} = \dots = 0.$$

(iv) Compute the new approximation

$$U^{(k+1)} = U^{(k)} + \alpha_k p^{(k)},$$

$$\text{where } \alpha_k = - \frac{(f^{(k)}, z^{(k)})}{(p^{(k)}, Jp^{(k)})}$$

and J is the Jacobian matrix $(\partial f_{i,j} / \partial U_{r,s})$ evaluated at $U^{(k)}$. In our experiments we choose the restart parameter to be $m = 9$, as in [8], and we continue the iteration until $\|f^{(k)}\|_2 \leq \text{EPS}$, where EPS is the desired tolerance.

We choose the matrix M in step (ii) to be one that approximates J in some sense and for which a fast-direct method can be used to solve $Mz^{(k)} = -f^{(k)}$. Our choice is the discrete Helmholtz operator scaled by a

diagonal matrix (see [8]). Specifically, $M = D^{1/2}(-2\Delta_h + KI)D^{1/2}$, where D is a diagonal matrix whose entries are $(\partial f_{i,j}/\partial U_{i,j} - 2Bh^2)/[2 \text{ diag } (-\Delta_h)]$, and $2\Delta_h$ is twice the discrete five-point Laplace operator on a mesh of width h , obtained by setting $W \equiv 1$ in the discrete form of (1), (2). We make the choice $K = 2Bh^2$, so that M is identical to the discrete form of (1), (2) when $W \equiv 1$.

To solve $Mz^{(k)} = -f^{(k)}$, we follow steps a to c below:

(a) Compute $-D^{-1/2}f^{(k)}$.

(b) Use a fast solver to find χ , where

$$(-2\Delta_h + 2Bh^2)\chi = -D^{-1/2}f^{(k)}.$$

(c) Compute $z^{(k)} = D^{-1/2}\chi$.

The multiplication of $Jp^{(k)}$ in the calculation of α_k in step (iv) of the algorithm is carried out utilizing fully the sparsity of J . Since J is block tridiagonal and each block is itself tridiagonal the multiplication takes less than $9(N+1)^2$ operations.

In the table below, we list the number of iterations to obtain $\|f^{(k)}\|_2 \leq \text{EPS}$ for different γ and B with $h = 1/40$, $\text{EPS} = 10^{-6}$, and $H \equiv 1$.

Table 4. Number of iterations required for convergence for $h = 1/40$
and $U^{(0)} \equiv 0$.

$\gamma \backslash B$	100	1	0.1	0.01
$\pi/4$	13	22	28	40
$\pi/3$	8	10	10	10

Each iteration takes approximately .139 sec., which includes .073 sec. for the fast solver, except for the first iteration, which requires 0.183 sec. including preprocessing. The program GMA (with parameter $K=2$) [2] was used to obtain the fast solution of Helmholtz's equation in our experiments. Notice that the dependence on the value of γ in Table 4 is much stronger than it is for the BSOR-Newton method. The smaller the angle, the more nonlinear the problem, and the more iterations required because M is less good an approximation to J and hence to f . Here, the value of B also influences the number of iterations required for convergence, more so in the case $\gamma = \pi/4$, for which W becomes very large near the corner $(0,0)$. The singular case $B=0$ can also be handled by this method when used with an appropriate fast solver.

2.3. Comparisons

We summarize the data from some of our experiments in the following tables. In all cases the initial approximation $U^{(0)} \equiv 0$ is used and the number of iterations given are those required to obtain a residual $\|f^{(k)}\|_2 \leq \text{EPS}$.

It appears, from the data in Tables 5 and 6, that the hybrid conjugate gradient method performs consistently better in terms of computer time for the model problem than does the block overrelaxation-Newton method. The conjugate gradient method has the further advantage of not requiring the estimation of an acceleration parameter such as ω (the dependence on the value of the restart parameter m is not as significant), and it is

Table 5. Number of iterations (CPU seconds) for the BSOR-Newton iteration

h	B	γ	Estimated ω		ω after 20 iterations	EPS=			
			best ω	for first 20 iterations		10^{-3}	10^{-4}	10^{-5}	10^{-6}
$\frac{1}{40}$	100	$\pi/3$	1.58	1.6	1.6	21(1.13)	29(1.56)	37(1.99)	44(2.36)
	100	$\pi/4$	1.59	1.5	1.55	25(1.34)	34(1.83)	43(2.31)	51(2.74)
	1	$\pi/3$	1.84	1.5	1.84	79(4.24)	98(5.26)	116(6.22)	>120(6.44)
	1	$\pi/4$	1.84	1.5	1.84	77(4.13)	90(4.83)	107(5.74)	>120(6.44)
	.01	$\pi/3$	1.85	1.5	1.8	116(6.22)	>120(6.44)		
	.01	$\pi/4$	1.85	1.5	1.8	118(6.33)	>120(6.44)		
$\frac{1}{20}$	100	$\pi/3$	1.52	1.2	1.5	15(.21)	20(.28)	24(.34)	27(.38)
	100	$\pi/4$	1.52	1.2	1.5	15(.21)	22(.31)	24(.34)	27(.38)
	1	$\pi/3$	1.71	1.5	1.7	46(.64)	56(.78)	66(.92)	76(1.06)
	1	$\pi/4$	1.71	1.5	1.7	46(.64)	55(.77)	65(.91)	75(1.05)
	.01	$\pi/3$	1.81	1.5	1.8	48(.67)	58(.81)	66(.92)	79(1.11)
	.01	$\pi/4$	1.82	1.5	1.8	49(.69)	58(.81)	67(.94)	79(1.11)

TABLE 6. Number of iterations (CPU seconds) for the conjugate gradient iteration

h	B	γ	EPS=			
			10^{-3}	10^{-4}	10^{-5}	10^{-6}
$\frac{1}{40}$	100	$\pi/3$	4(.60)	5(.74)	6(.88)	8(1.16)
	100	$\pi/4$	6(.79)	8(1.16)	10(1.44)	13(1.90)
	1	$\pi/3$	5(.74)	7(1.02)	8(1.16)	10(1.44)
	1	$\pi/4$	13(1.90)	15(2.18)	18(2.59)	22(3.19)
	.01	$\pi/3$	5(.74)	6(.88)	8(1.16)	10(1.44)
	.01	$\pi/4$	15(2.18)	29(4.16)	34(4.91)	40(5.74)
$\frac{1}{20}$	100	$\pi/3$	4(.14)	5(.17)	6(.21)	7(.24)
	100	$\pi/4$	5(.17)	6(.21)	7(.24)	9(.30)
	1	$\pi/3$	5(.17)	7(.24)	8(.27)	9(.30)
	1	$\pi/4$	10(.34)	14(.48)	16(.54)	19(.64)
	.01	$\pi/3$	5(.17)	6(.21)	8(.27)	9(.30)
	.01	$\pi/4$	13(.44)	22(.74)	25(.84)	35(1.18)

less sensitive to the initial approximation, although it does require more computer storage than is required for the BSOR-Newton method [8]. For nonrectangular domains the conjugate gradient method would lose some of its competitive advantage of speed since more computer time is required by fast-direct methods in this case for the solution of the Helmholtz equation. See [8] for other possible choices for M and for comparisons of the conjugate gradient method with the BSOR-Newton method for the case $B = H = 0$ with boundary conditions for which the problem is not singular.

In order to estimate the discretization error, the numerical solution for $B=0$, $\gamma = \pi/4$, $h = 1/20$ was compared with the known closed-form solution. We found the relative error of the computed solution in the infinity norm to be less than about 1/2% everywhere beyond 3 grid points from the corner, 18% right at the corner, and 1 to 4% in between. The relative difference between the computed solutions on the grids for $h = 1/40$ and $h = 1/20$ was about 2% in the infinity norm for this case.

3. The unbounded case

As pointed out in Sec. 1, there is a critical contact angle γ_0 , which is $\pi/4$ for our model problem, such that the solution is unbounded at the corner of the cylinder cross section for all $\gamma < \gamma_0$. The asymptotic form of the solution in a neighborhood of the corner is given by (3). If $\gamma < \gamma_0$, we use this asymptotic solution in conjunction with discrete methods away from the corner to solve our problem.

We investigate two methods that use different discretization procedures over the portion of the domain away from the corner. In the first method, a neighborhood of the corner is deleted entirely from the domain to be discretized. In the second, the asymptotic solution is extended into part of this domain. We consider, as in the previous section, only the model problem of a square on which has been placed a uniform square mesh.

3.1. Method A

Here we assume that the asymptotic behavior (3) holds from the vertex of the corner with the singularity up to one or several grid points away. We term this portion of the domain the asymptotic domain and the remaining portion the numerical domain (see figure 3).

A natural way to obtain the numerical domain is to cut along a level curve of the asymptotic solution. The analytical solution in this domain then can provide an upper bound on the solution u of (1),(2) [9]. Although the level curves of the asymptotic solution are circular arcs, the limitations of our experimental computer program require us to approximate such an arc by a straight line passing through mesh points and making an angle of 45° with the edges of the square. Thus, we solve equations (1) and (2) numerically in the domain shown in figure 4.

The boundary conditions of the previous section apply at all boundary points, except those on Γ , where we use a normal-derivative matching condition obtained by differentiating (3). After solving the resulting problem in the numerical domain, we can obtain a value for $v - u$ in the

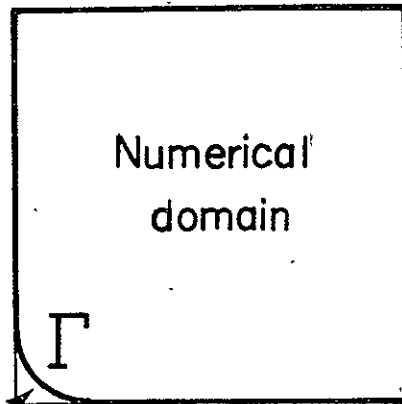


Fig. 3

Division of the domain for Method A.

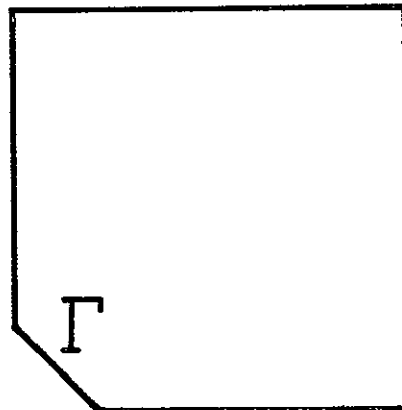
Asymptotic
domain

Fig. 4

The numerical domain for the test
problem.

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asymptotic domain by matching at one (or more) points of Γ . In this way, we obtain an approximation to the solution over the entire domain Ω .

We use the same discrete equation(5) at a general interior point of the numerical domain as in Sec. 2.1. On Γ , the discrete equation at a general point is (see figure 5)

$$f_{i,j} = W_{\bar{i}+1,\bar{j}+1}^{-1} \begin{pmatrix} 2U_{i,j} & -U_{i+1,j} & -U_{i,j+1} \end{pmatrix} W_{\bar{i},\bar{j}+1}^{-1} \begin{pmatrix} U_{i,j+1} & -U_{i,j} \end{pmatrix} \\ - W_{\bar{i}+1,\bar{j}}^{-1} \begin{pmatrix} U_{i+1,j} & -U_{i,j} \end{pmatrix} \\ - 2 \int_{\Gamma_i} \frac{1}{W} \frac{\partial U}{\partial n} d\ell + h^2 \left(BU_{i,j} + 2H \right) = 0,$$

where

$$W_{\bar{i},\bar{j}+1} = \left[1 + \left(U_{i,j+1} - U_{i-1,j+1} \right)^2 / h^2 + \left(U_{i,j+1} - U_{i,j} \right)^2 / h^2 \right]^{1/2}, \\ W_{\bar{i}+1,\bar{j}} = \left[1 + \left(U_{i+1,j} - U_{i,j} \right)^2 / h^2 + \left(U_{i+1,j} - U_{i+1,j-1} \right)^2 / h^2 \right]^{1/2},$$

and $\int_{\Gamma_i} \frac{1}{W} \frac{\partial U}{\partial n} d\ell$ is evaluated by Simpson's rule using the directional

derivative from (3) for the values of $W^{-1} \partial v / \partial n$,

$$\left. \frac{1}{W} \frac{\partial U}{\partial n} \right|_{\Gamma} = \frac{-a_1(x+y) + a_2(y-x)}{\left[2(x^2+y^2)(1+a_1^2+a_2^2) \right]^{1/2}}, \quad (6)$$

where

$$a_1 = - \left(\cos \theta - \left[\kappa^2 - \sin^2 \theta \right]^{1/2} \right) / (\kappa B \rho^2)$$

$$a_2 = \left(\sin \theta \cos \theta \left[\kappa^2 - \sin^2 \theta \right]^{-1/2} - \sin \theta \right) / (\kappa B \rho^2)$$

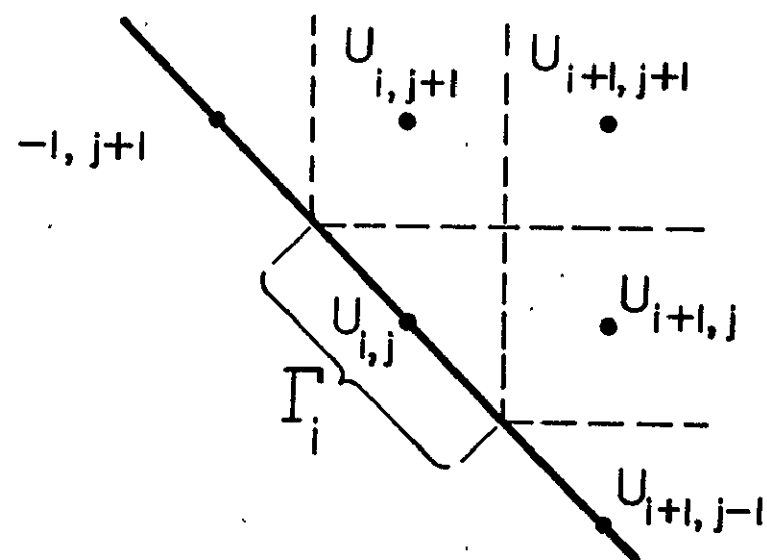
$(\theta, \kappa, B, \rho$ as defined in (3)).

The discrete equation for points one mesh interval away from Γ in the interior of the numerical domain is the same as (5), except that for (i, j) on Γ , $W_{\bar{i}, \bar{j}}$ is given by $W_{\bar{i}, \bar{j}} =$

$$\left(1 + (U_{i,j} - U_{i,j-1})^2/h^2 + (U_{i,j} - U_{i-1,j})^2/h^2 \right)^{1/2}.$$

We consider only the BSOR-Newton method for solving the discretized equations in the numerical domain. General purpose programs for solving the discrete Helmholtz equation are being developed and were not available for use with the conjugate gradient method during our study. These programs require, in general, more computer time than ones for a rectangular domain.

The determination of how far into the domain Γ should be placed for optimal accuracy poses an essential difficulty for the method: If



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Fig. 5

The boundary points of Γ .

Γ is too far into the domain, the boundary condition obtained from the asymptotic representation on Γ will be inaccurate; if Γ is too close to the corner, the discretization in the numerical domain near Γ may not be able to represent well the steepness of the solution. Considering these two alternatives, it appears that it is better to put Γ close to the corner, because one can, in principle, always refine the mesh locally or use higher-order or other methods to handle the steepness of the solution, while errors committed by pushing Γ too far into the domain cannot be compensated for easily.

In our numerical experiments, we choose Γ to be sufficiently close to the corner so that at p , the midpoint of Γ , $W^{-1}\partial v/\partial n \geq 0.999 \doteq \cos^{-1} 2.5^\circ$. We solve the resulting problem on the numerical domain with a mesh size h of $1/40$ and $1/80$, to give an indication of the discretization error for the particular choice of Γ . We also solve problems for nearby choices of Γ to determine the sensitivity to the positioning of Γ .

Of course, the matching conditions (6) on Γ may not be accurate. Although the difference between u and the asymptotic solution v is bounded by a constant as the corner is approached, the difference between their derivatives may be large. If Γ is chosen to be an actual level curve of v , close enough to the vertex so that $|\nabla v|$ is large and $W^{-1}\partial v/\partial n$ is essentially 1 there, then $|\nabla u|$ would also be large and choosing $W^{-1}\partial u/\partial n$ to be essentially 1 along Γ should then be sufficiently

accurate to be in keeping with the discretization errors in the interior. However, along the straight-line approximation to the level curve required by our test program, $W^{-1}\partial v/\partial n$ can vary appreciably, and attempting to match to $W^{-1}\partial u/\partial n$ as in (6) might lead to errors. Our goal is to obtain from our experimental program not necessarily solutions of the highest accuracy but rather an indication of the feasibility of our use of the asymptotic solution (3) near the corner singularity in conjunction with a discrete method elsewhere.

We give here a summary of some of the typical behavior found in our numerical experiments.

For the case $\gamma = 0^\circ$, $B = 1$, and Γ at the position where $W^{-1}\partial v/\partial n|_p \doteq 0.999$ (i.e., Γ is on the 17th grid point of the first row in an 81×81 mesh, or the 9th grid point of the first row in a 41×41 mesh), moving Γ one grid point in the 81×81 mesh produces less than .1% relative difference in the solution in the interior 90% of the domain, between .1% and 1% relative difference in a band closer to Γ covering about 7% of the domain, and between 1% and 3.5% for the points in the immediate neighborhood of Γ . The relative difference is correspondingly about twice as much in the 41×41 case when Γ is moved by one mesh point. The relative difference in the solution resulting from refining the mesh from $1/40$ to $1/80$, keeping Γ fixed, is less than 0.2% over the interior 50% of the domain, between 0.2% and 1% over 30% of the domain, between 1% and 5% over 10% of the domain, and between 5% and 15% on the points in the immediate neighborhood of Γ .

For $\gamma = 30^\circ$, $B = 1$, and $W^{-1}\partial v/\partial n|_p \doteq 0.999$, the relative differences are about one-fourth of those of the above experiments for $\gamma = 0^\circ$.

Less sensitivity is to be expected because the solution surface is generally not as steep in this case. For similar reasons, the case for $\gamma = 0^\circ$, $B = 10$, $W^{-1}\partial v/\partial n|_p \doteq 0.999$, has about only half of the relative differences found for the case $\gamma = 0^\circ$, $B = 1$.

If we choose Γ so that $W^{-1}\partial v/\partial n|_p \doteq 0.9999$, then the relative differences from refining the mesh were found to be two to three times as large as they were for placing Γ at a position for which $W^{-1}\partial v/\partial n|_p \doteq 0.999$.

Based on the above information, we choose Γ so that $W^{-1}\partial v/\partial n|_p \doteq 0.999$ for most of our experiments.

For the case of $\gamma = 0^\circ$, $B = 1$, the solution height in the numerical domain was found to be $U|_p \doteq 1.46$ for the 81×81 grid. We compare solution heights obtained from placing Γ on the 9th grid point on the first row (in this case, $W^{-1}\partial v/\partial n|_p \doteq 0.9999$) and placing Γ on the 17th grid point on the first row (in this case, $W^{-1}\partial v/\partial n|_p \doteq 0.999$) on a 81×81 grid. Although rather large relative differences exist for points close to Γ , we observe that over 75% of the domain less than a 1% change occurs. This indicates that the solution over a large portion of the domain is rather insensitive to where Γ is placed. As mentioned previously, over the same large portion, refining the mesh from $1/40$ to $1/80$ also produces only minor changes. Thus, for that portion of the domain, a medium size mesh (say, $h = 1/40$) seems sufficient to produce acceptably

accurate results. We observe also that for fixed Γ the numerical solution appears to be converging as h tends to zero through the different mesh sizes.

For the unbounded case, the convergence of the BSOR-Newton method is even more sensitive to changes of ω than for the bounded case, especially for $\gamma = 0^\circ$. For $U^{(0)} \equiv 0$, one must begin the iteration with ω close to 1 to prevent divergence, and then quickly (within 20 iterations, say) increase ω toward the estimated optimal value in order to obtain an acceptably rapid convergence rate. Overestimating ω essentially always leads to divergence. For $\gamma = 0^\circ$, the observed optimal values of ω found experimentally are listed in Table 7.

Table 7. Observed optimal ω for $\gamma = 0^\circ$.

$\begin{array}{c} B \\ \backslash \\ h \end{array}$	1	10	100
1/20	1.70	1.61	1.33
1/40	1.84	1.78	1.50
1/80	1.92	1.88	not available

The optimal values of ω for $\gamma = 30^\circ$ are about the same as for $\gamma = 0^\circ$. One can see from Table 7 that both the grid size and value of B influence the value of the optimal ω .

Table 8 summarizes our experimental results for a range of values of γ , B , and h . The number of iterations

TABLE 8. Number of iterations (CPU seconds) for method A

γ	B	h	Γ^*	Initial [†] approx.	ω		ω_{opt} (estimated)	DEL =			
					starting	after 20 steps		10^{-3}	10^{-4}	10^{-5}	10^{-6}
0	1	$\frac{1}{20}$	4	S	1.5	1.69	1.70	31(.46)	42(.63)	51(.76)	61(.91)
0	1	$\frac{1}{40}$	8	S	1.79	1.84	1.84	37(2.04)	56(3.08)	71(3.91)	85(4.68)
0	1	$\frac{1}{80}$	16	S	1.79	1.84**	1.92	70(16.1)	112(25.76)	170(39.10)	
0	10	$\frac{1}{20}$	1	0	1.5	1.59	1.61	24(.35)	33(.49)	41(.61)	48(.72)
0	10	$\frac{1}{40}$	1	0	1.55	1.75	1.78	46(2.53)	64(3.53)	81(4.46)	97(5.34)
0	10	$\frac{1}{80}$	4	0	1.55	1.79 ^{††}	1.89	90(20.70)	141(32.43)	178(40.94)	
$\frac{\pi}{6}$	1	$\frac{1}{20}$	3	S	1.5	1.69	1.71	24(.36)	38(.57)	48(.71)	59(.88)
$\frac{\pi}{6}$	1	$\frac{1}{40}$	6	S	1.79	1.84	1.84	26(1.43)	50(2.75)	68(3.74)	84(4.62)
$\frac{\pi}{6}$	10	$\frac{1}{20}$	1	0	1.5	1.59	1.61	25(.37)	34(.51)	42(.63)	50(.75)
$\frac{\pi}{6}$	10	$\frac{1}{40}$	1	0	1.55	1.75	1.78	48(2.64)	66(3.64)	84(4.63)	102(5.62)

* The number of grid intervals from the corner at which Γ meets an edge of Ω .

** $\omega = 1.9$ after 100 iterations.

[†] 0 - identically zero; S-portion of a sphere (i.e. exact solution for $B=0$, $\gamma=\pi/4$).

^{††} $\omega = 1.87$ after 100 iterations.

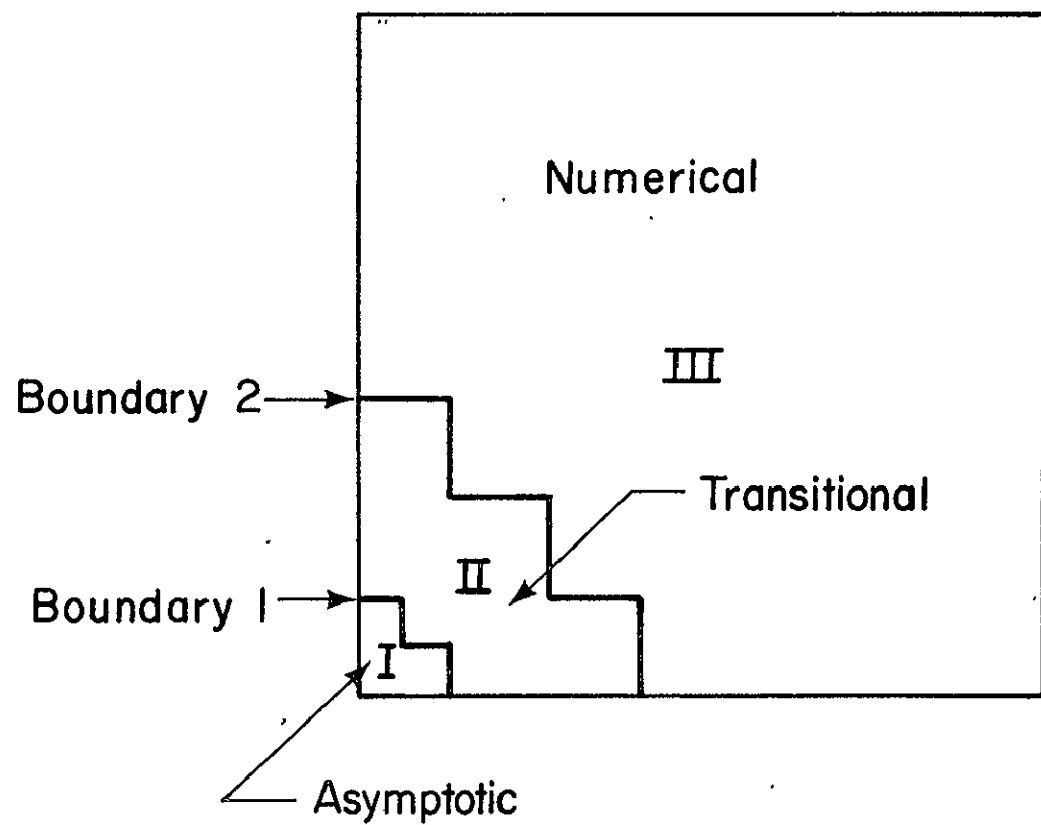
given in Table 8 are those required for $\|u^{(k)} - u^{(k-1)}\|_2 / \|u^{(k)}\|_2 \leq \text{DEL}$.

A major difficulty for this method is the representation of the steep gradients of the solution in the numerical domain near Γ . In the next section, we investigate the possibility of handling this difficulty by overlapping a portion of the numerical with the asymptotic domain.

3.2. Method B

Here we investigate the possibility of improving the previous method by overlapping the asymptotic and numerical solutions over part of the domain. We divide the entire domain into the three regions shown in Figure 6. Region I is a small portion of the domain near the corner in which we assume that the asymptotic behavior (3) holds. Region III, including boundary 2 in Figure 6, is the purely numerical domain, in which we assume that the solution u is not too steep and can be computed accurately with the discretization used previously. The region between is Region II, where we couple the asymptotic and numerical solutions under the assumption that u and v differ there by a lower-order quantity that is not steep and thus can be computed more accurately with a discretization than can either u or v . The staircase-shaped domain boundaries are used rather than the 45° lines of Method A to approximate level curves because the limitations of our study permitted us to use only those boundaries that were simplest to include in the computer program.

Let u be the solution to (1) and (2), then in Region I and II we



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Fig. 6

The three regions for Method B.

write $u = v + \varepsilon$, where v is given by the asymptotic expression (3) and $|\varepsilon|$ is bounded by a constant. Over Region II, we consider $\varepsilon(x,y) = u(x,y) - v(x,y)$ and we derive discrete equations for $\varepsilon(x,y)$ involving the known quantity v , keeping only the first-order terms in ε/v and in the derivatives of ε divided by those of v . Over Region I, we take $\varepsilon = \varepsilon_0$, as in Method A, where ε_0 and its derivatives are negligible compared with v and its derivatives.

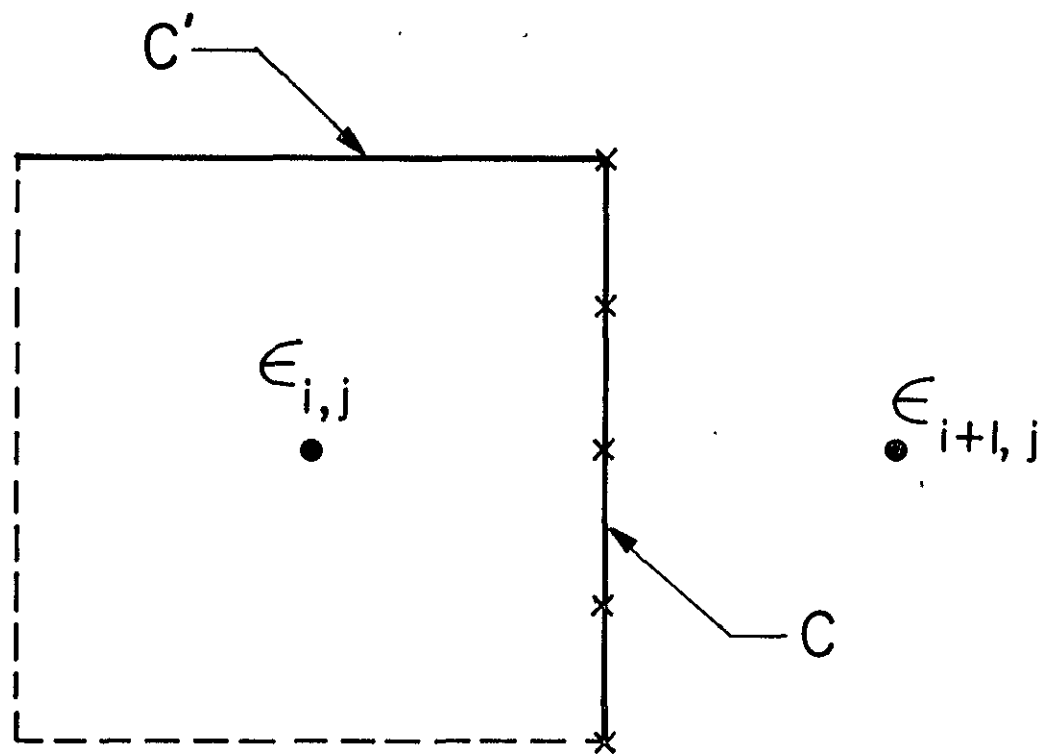
In Region II, the left hand side of (4) becomes

$$\begin{aligned} & \int_{\partial D} \frac{(v + \varepsilon)_n}{\left[1 + (v_x + \varepsilon_x)^2 + (v_y + \varepsilon_y)^2\right]^{1/2}} d\ell \\ &= \int_{\partial D} \frac{(v + \varepsilon)_n}{\left[1 + v_x^2 + v_y^2\right]^{1/2}} \left[1 + \frac{-v_x \varepsilon_x - v_y \varepsilon_y}{\left(1 + v_x^2 + v_y^2\right)} + O\left(\frac{\varepsilon_x^2 + \varepsilon_y^2}{v_x^2 + v_y^2}\right)\right] d\ell. \end{aligned} \quad (7)$$

When we perform the integration along a direction parallel to y-axis, then the normal direction in (7) is parallel to the x-axis, and the right-hand side of (7) becomes (see figure 7)

$$\int_C \frac{v_x d\ell}{\left[1 + v_x^2 + v_y^2\right]^{1/2}} + \int_C \varepsilon_x \frac{1 + v_y^2}{\left[1 + v_x^2 + v_y^2\right]^{3/2}} d\ell - \int_C \varepsilon_y \frac{v_x v_y}{\left[1 + v_x^2 + v_y^2\right]^{3/2}} d\ell \quad (7a)$$

+ higher order terms.



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Fig. 7

Integration path on an auxiliary mesh cell boundary

If the normal direction $\underline{n}$ is parallel to the y-axis, as along C' , then the right-hand side of (6) becomes

$$\int_{C'} \frac{v_y d\ell}{[1+v_x^2+v_y^2]^{1/2}} + \int_{C'} \epsilon_y \frac{1+v_x^2}{[1+v_x^2+v_y^2]^{3/2}} d\ell - \int_{C'} \frac{v_x v_y}{[1+v_x^2+v_y^2]^{3/2}} d\ell \quad (7b)$$

+ higher order terms.

To form discrete equations for $\epsilon_{i,j}$, we evaluate (7a) along C , for example, by using Simpson's rule with the five indicated node points for computing the three integrals involving v , with ϵ_x replaced by

$(\epsilon_{i+1,j} - \epsilon_{i,j})/h$ and ϵ_y replaced by $(\epsilon_{i,j-1} - \epsilon_{i,j} + \epsilon_{i+1,j+1} - \epsilon_{i+1,j})/2h$

for the upper half of C and by $(\epsilon_{i,j} - \epsilon_{i,j-1} + \epsilon_{i+1,j} - \epsilon_{i+1,j-1})/2h$

for the lower half of C . If we then ignore terms that contain powers

greater than one of ϵ/v and of the ratio of their derivatives, we obtain

a system of linear equations for $\epsilon_{i,j}$. The associated matrix is symmetric

and banded.

3.2.1. The iteration

In solving the discrete equations in Region II, the boundary condition on boundary 1 is obtained from the directional derivative of the asymptotic formula (3), and the boundary condition at each iteration for boundary 2 is obtained by keeping the value of u fixed at its Region III value. We use the IMSL subroutine LEQTLB, designed to solve banded systems, to obtain the solution. Note that for the different boundary

conditions on boundary 2 arising from each iteration, only the right hand side of the system to be solved in Region II needs to be changed. Therefore, it is necessary to perform the associated triangular decomposition only for the first iteration.

The method of solution for Region III is the BSOR-Newton method of the previous sections. The boundary condition on boundary 2 is that of keeping the value of U (i.e. ϵ) fixed at its value obtained previously in Region II. Afterwards, we adjust the value of H in the same way as before, using the boundary of Region III as the contour for (3).

Each iteration thus consists of solving for ϵ in Region II followed by solving for U in Region III and then adjusting H .

3.2.2. Experimental Results

We have experimented with this method for $\gamma = 0^\circ$, $B = 1$ and $B = 10$ on a 41×41 grid. We took boundary 1 to intersect the edge of the square one grid point from the corner, and boundary 2 to intersect the edge at the 10th grid point for $B = 1$ and the 4th grid point for $B = 10$. We found the solutions generally insensitive to these boundaries being moved by one or two mesh intervals. The time required for convergence was about three times greater than for Method A.

Of importance is the observation, that in our experiments the value of $|\nabla \epsilon|$ obtained was not necessarily small compared with that of $|\nabla v|$. In fact, $|\nabla \epsilon|$ was almost half of $|\nabla v|$ for most points in Region II, including the points close to the vertex. Thus the assumption, on which the numerical scheme in Region II is based, that $|\nabla \epsilon| / |\nabla v|$ is small does not hold even though $|\epsilon| / |v| \rightarrow 0$ as the vertex is approached.

3.3. Conclusion

Since the results from Method B indicate that the assumption on which it is based does not generally hold, we conclude that Method B is not a suitable technique for improving Method A for this problem. The experimental results for Method A for the 21×21 , 41×41 , 81×81 grids, for a fixed position of Γ indicate convergence of the numerical solution as h (the mesh size) $\rightarrow 0$. In addition, the values of U on the bulk of the domain change very little as the mesh is refined, indicating that reasonable accuracy can be obtained away from the corner even for the coarser grids.

From the experimental data, it appears that taking Γ to be the line on which the value of v_n/W at the midpoint is about 0.999 is reasonably satisfactory. Moving Γ one or two mesh intervals produces less than 0.5% relative difference in the numerical solution over 90% of the grid points. As for the points close to Γ , one should consider using a finer mesh or higher-order discretization than in the rest of the domain and taking Γ to be a level curve of the asymptotic solution with an irregular mesh nearby. These matters are considered further in a related study [1].

In Figures 9 to 18, we present graphical computer output depicting perspective views with contours for some of the numerical solutions

that were obtained with the methods of Section 2 for the bounded case and with Method A for the unbounded case. The perspective views displayed are those indicated in figure 8. The height contours are drawn at intervals of 0.1, measured from the center (1,1) where the height is taken to be zero.

Solution surfaces for $B=1$ are depicted in figure 9 for $\gamma=60^\circ$ (a bounded case) and in figures 10 to 13 for $\gamma=30^\circ$ and $\gamma=0^\circ$ (unbounded cases). Those for $B=10$ are depicted in figure 14 for $\gamma=60^\circ$ and figures 15 to 18 for $\gamma=30^\circ$ and $\gamma=0^\circ$. All perspective views are at an inclination angle of 20° and a viewpoint distance of 100 units.

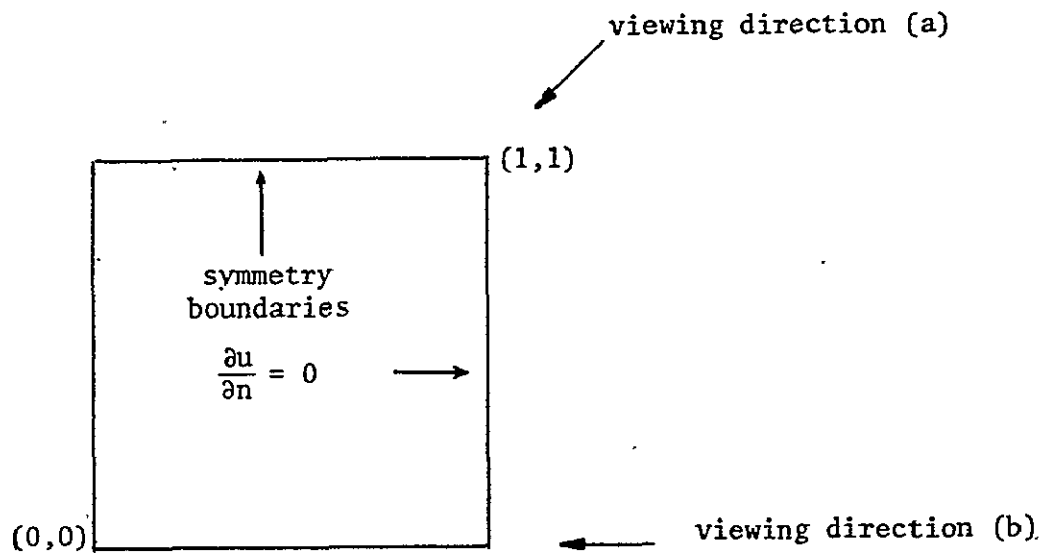


Figure 8

Test problem domain showing perspective
viewing directions.

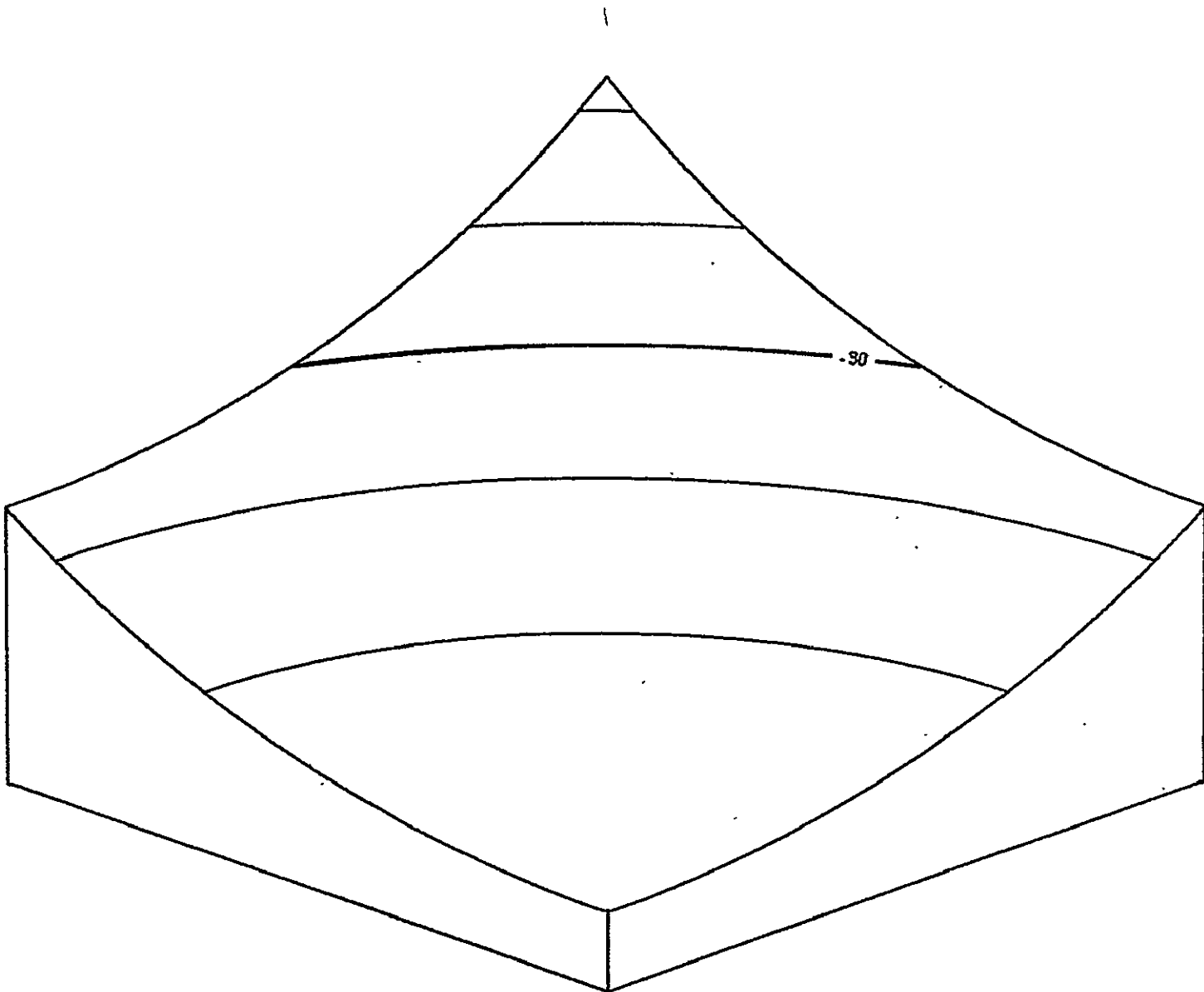


Figure 9
Perspective view for $B = 1$ from
direction (a), $\gamma = 60^\circ$.

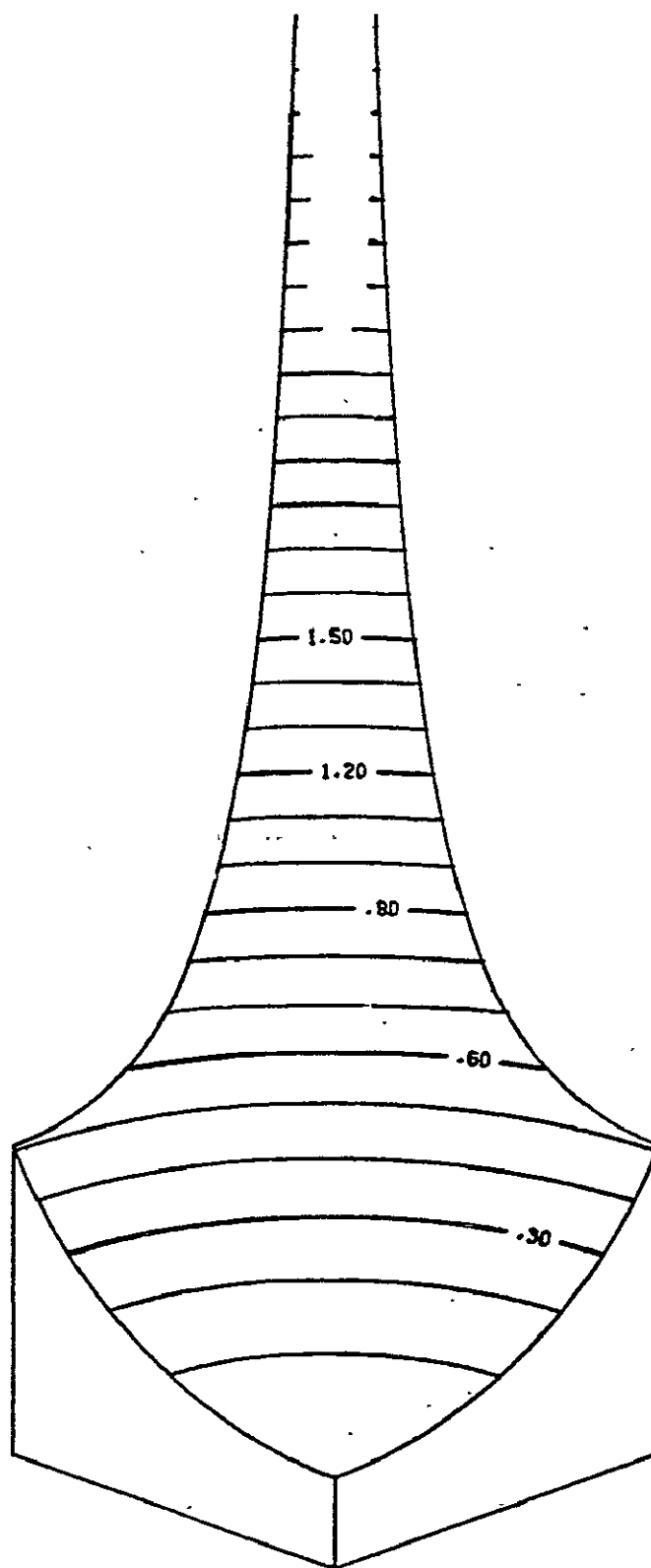


Figure 10. Perspective view for $B = 1$ from direction (a), $\gamma = 30^\circ$.

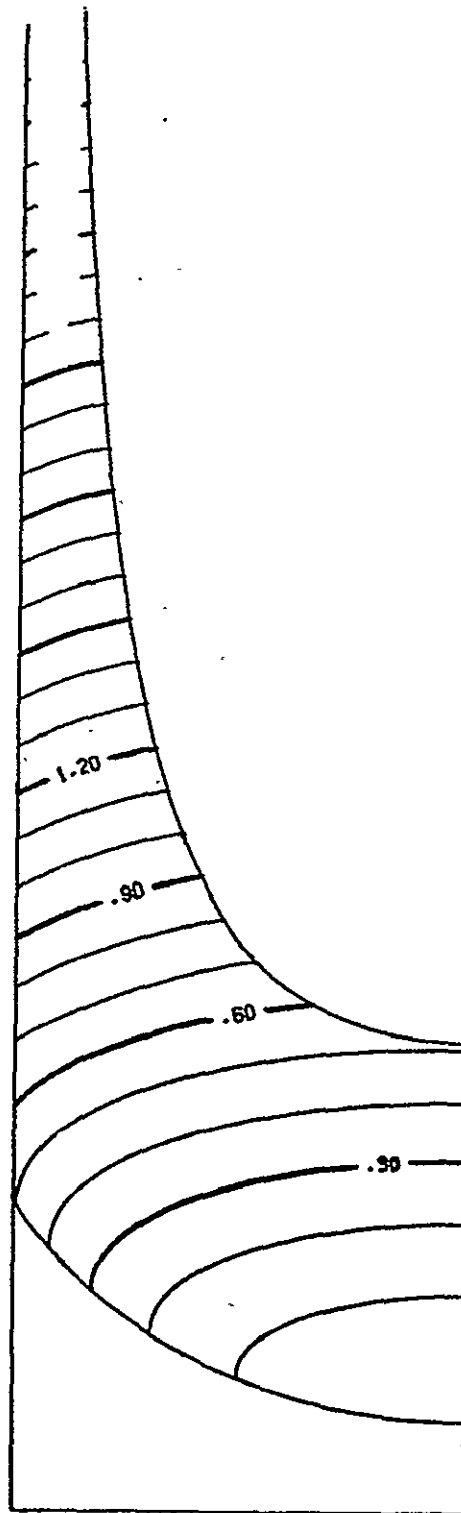


Figure 11. Perspective view for $B = 1$ from direction (b), $\gamma = 30^\circ$.

C2

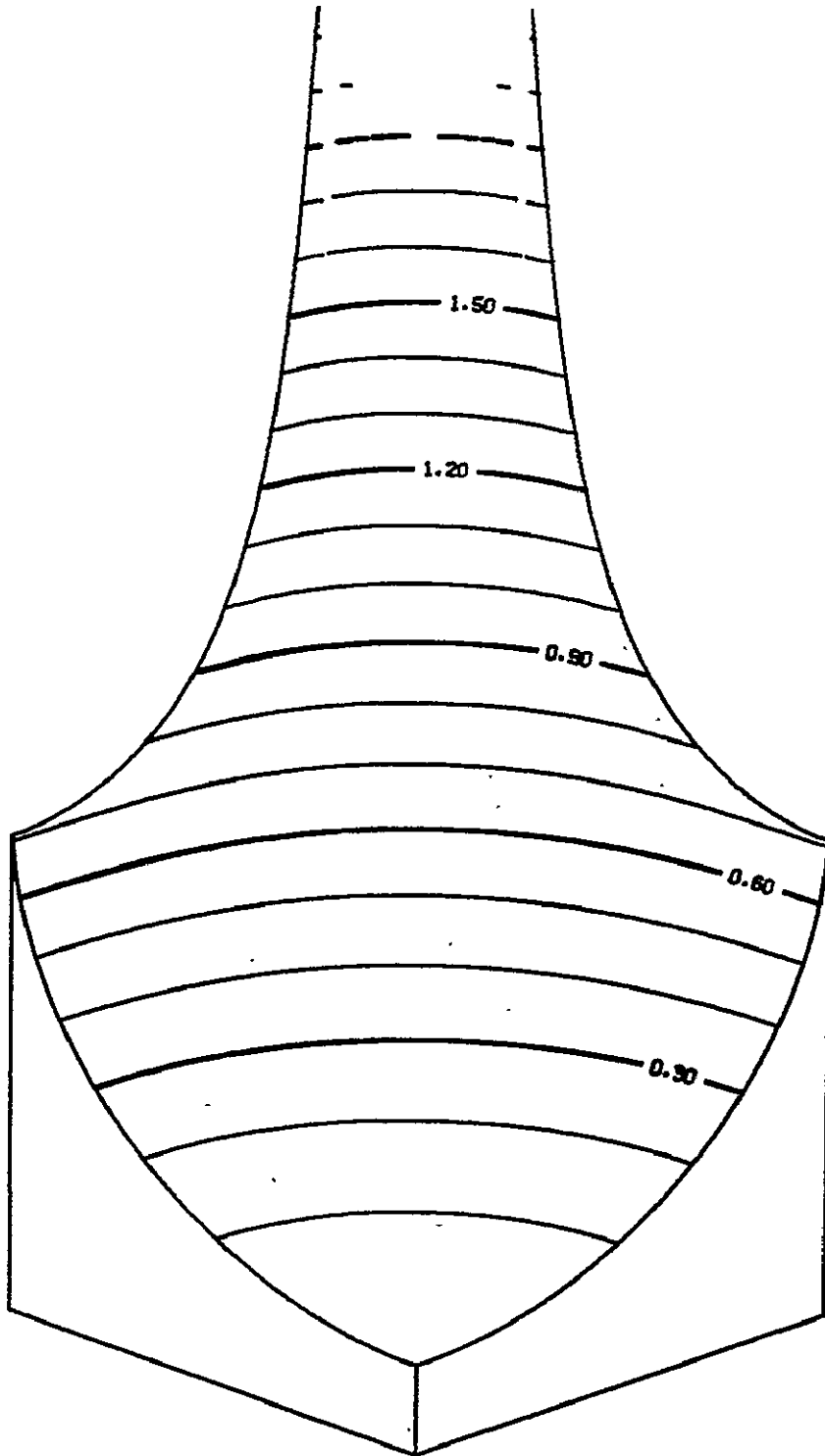


Fig. 12

Perspective view for $B = 1$ from direction (a), $\gamma = 0^\circ$.

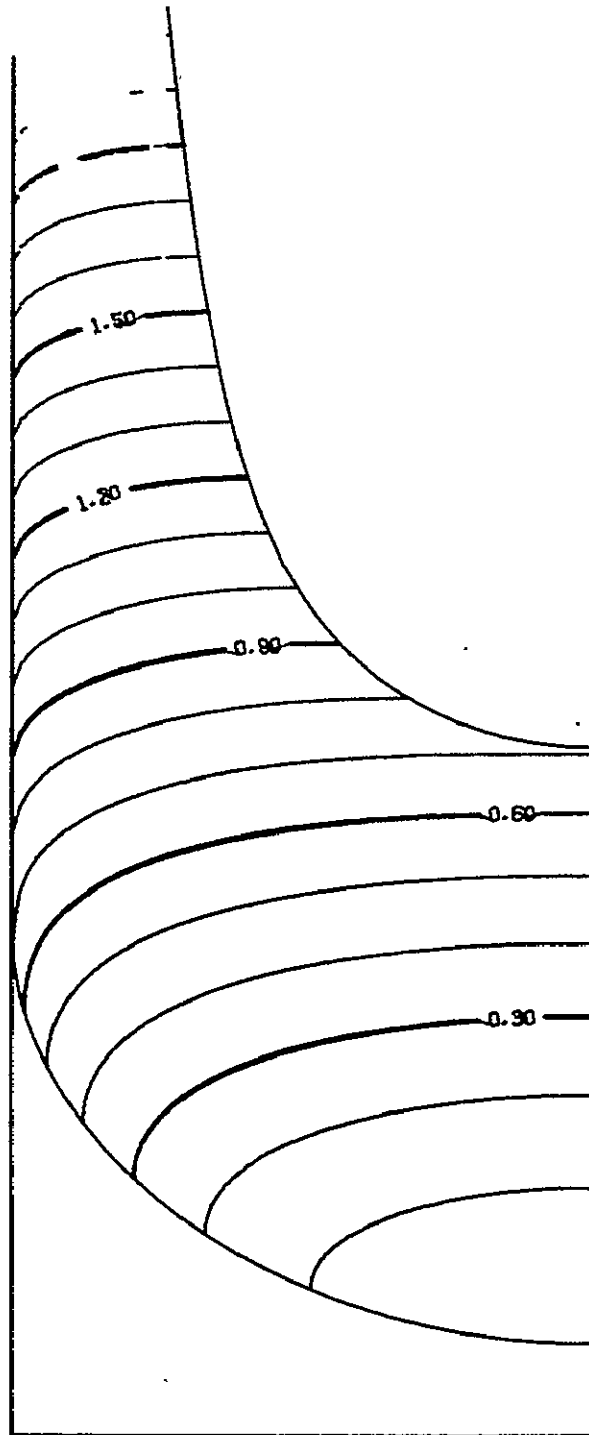


Fig. 13

Perspective view for $B = 1$ from direction (b), $\gamma = 0^\circ$.

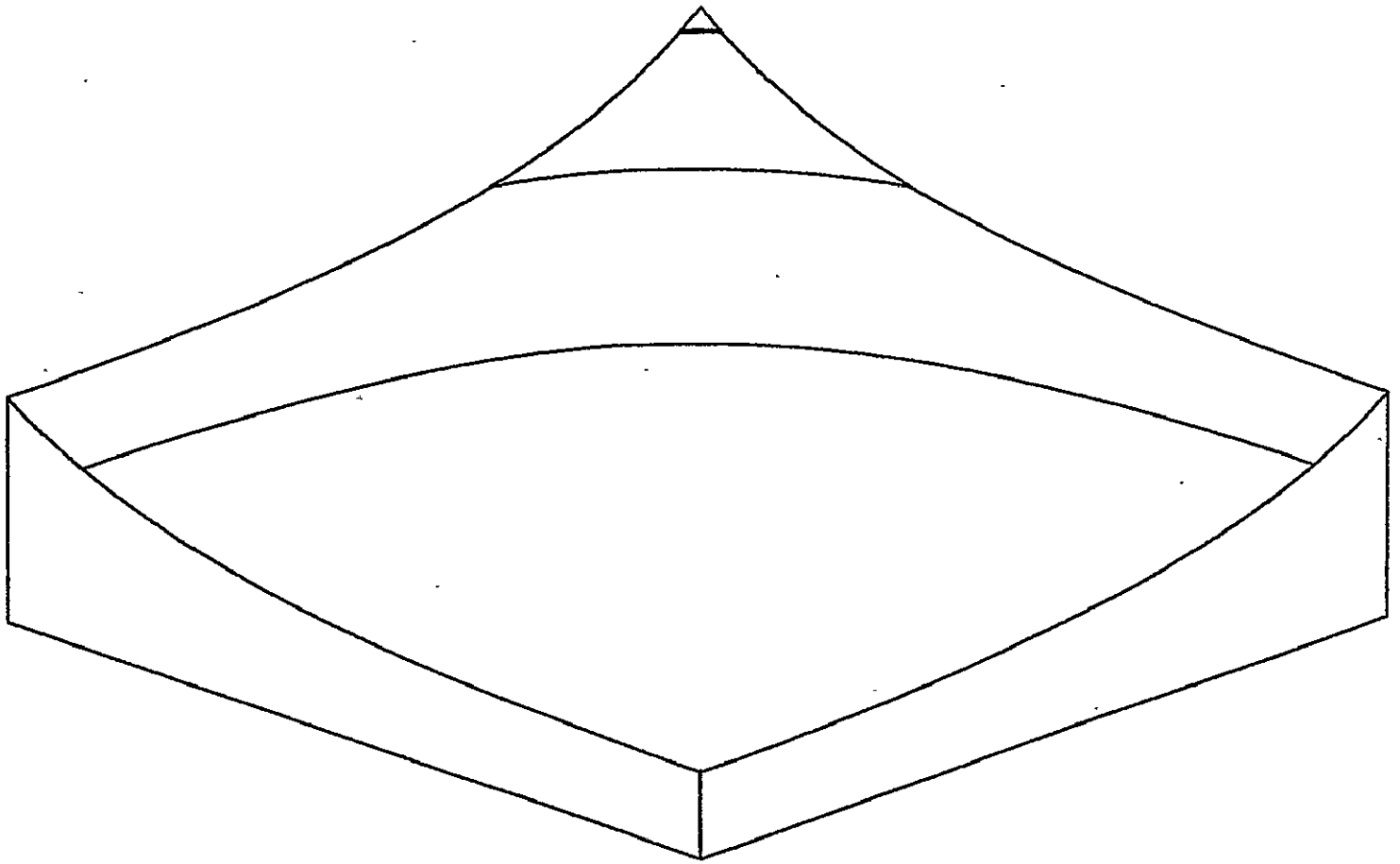


Figure 14

Perspective view for $B = 10$ from
direction (a), $\gamma = 60^\circ$.

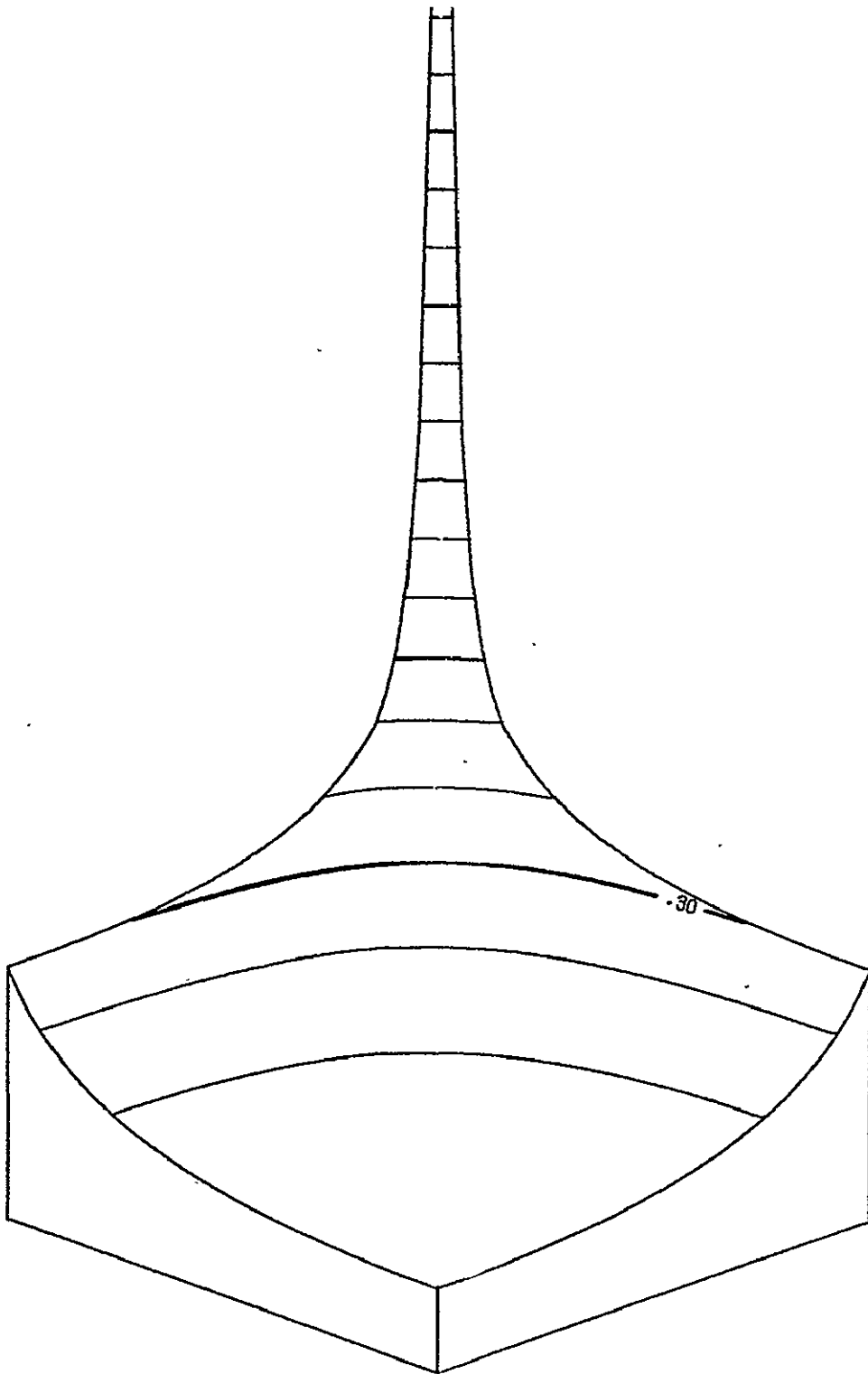


Figure 15

Perspective view for $B = 10$ from
direction (a), $\gamma = 30^\circ$.

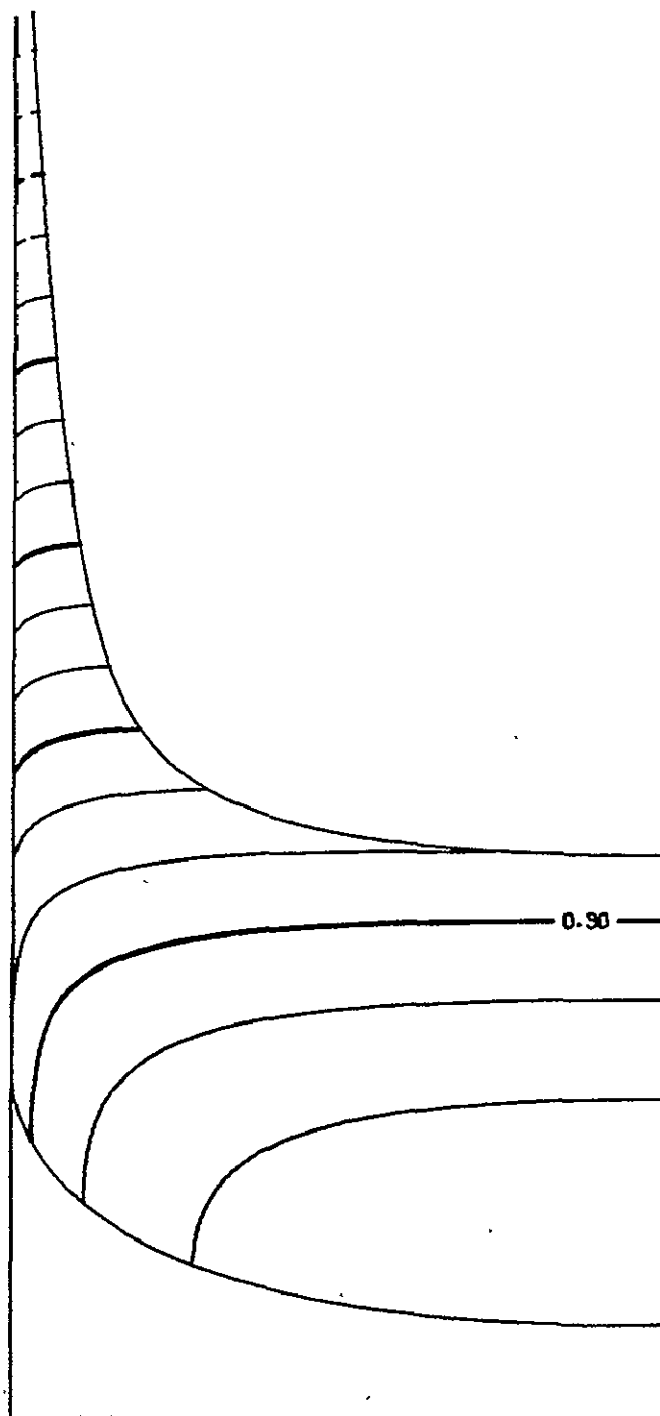


Fig. 16

Perspective view for $B = 10$ from direction (b), $\gamma = 30^\circ$.

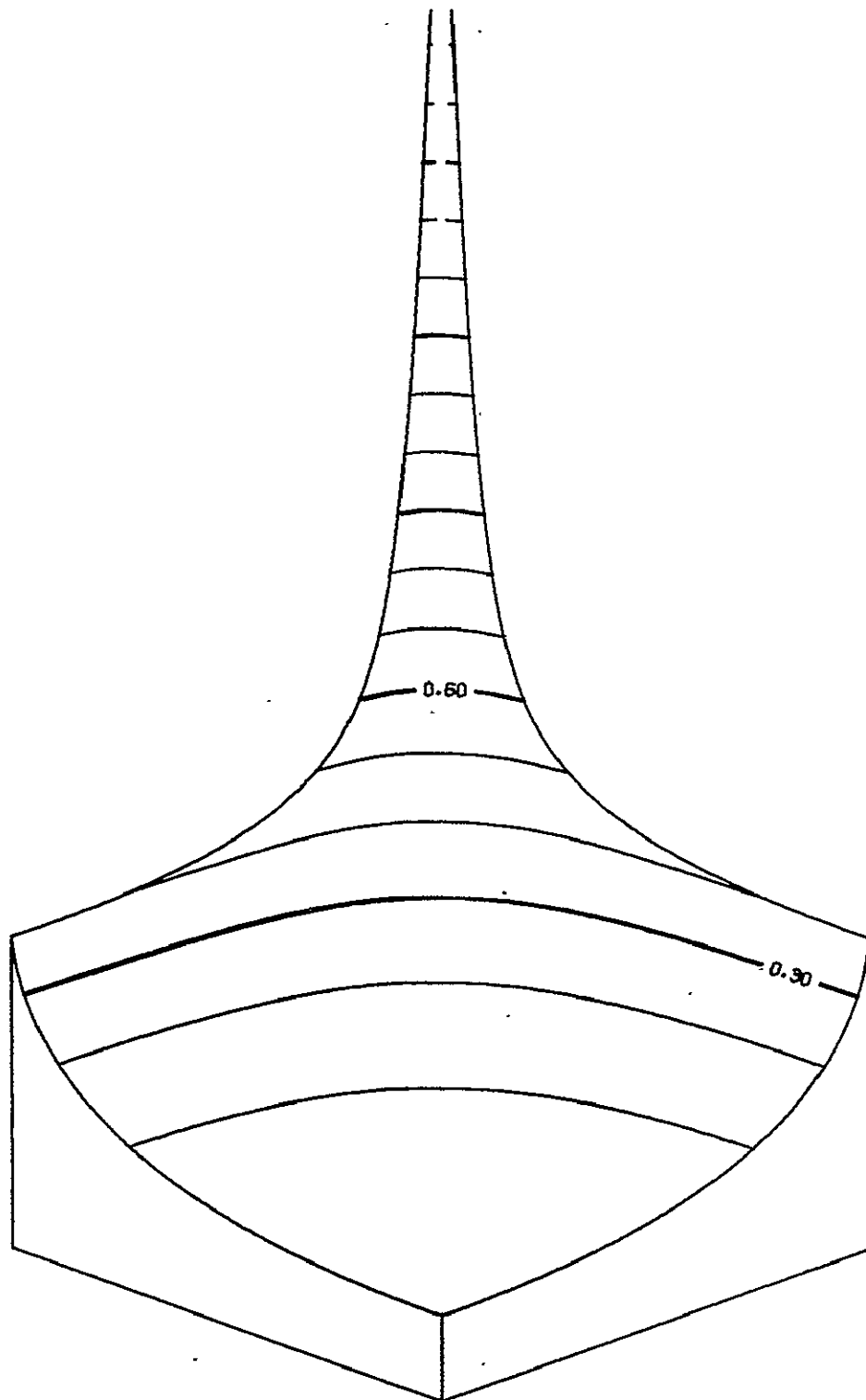


Fig. 17

Perspective view for $B = 10$ from direction (a), $\gamma = 0^\circ$.

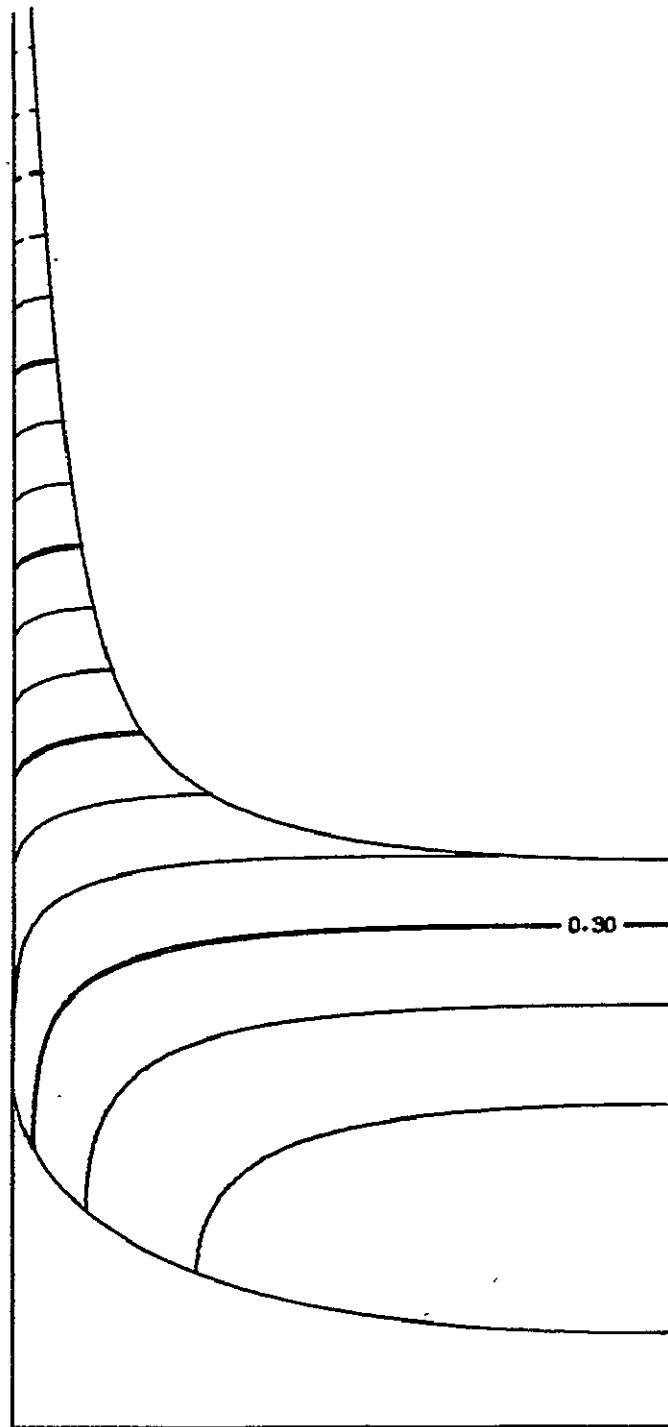


Figure 18

Perspective view for $B = 10$ from
direction (b), $\gamma = 0^\circ$

Acknowledgments

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APPENDIX IV

NUMERICAL COMPUTATION OF CAPILLARY SURFACES
ON IRREGULARLY SHAPED DOMAINS BY A FINITE
ELEMENT METHOD

by

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NUMERICAL COMPUTATION OF CAPILLARY SURFACES
ON IRREGULARLY SHAPED DOMAINS BY A
FINITE ELEMENT METHOD

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ABSTRACT

In this report we explore the nature of capillary surfaces on several noncircularly symmetric domains and investigate the suitability of the computer program JASON for calculating these surfaces. We investigate how the accuracy of the computed solution depends on various parameters. We calculate capillary surfaces for elliptical cross sections. We describe a procedure for calculating surfaces on cross sections with corners for values of the contact angle less than the critical value. We use this method to calculate surfaces on a square cross section and on a circular cross section with a reentrant notch.

1. INTRODUCTION

In this report we explore the nature of capillary surfaces on various noncircularly symmetry domains and investigate the suitability of the computer program JASON for calculating these surfaces.

In the next section we define the capillary surface problem for liquids with contact angle γ between 0° and 90° . The surface satisfies a pair of equations, Eqs. (1) and (2). In the following section we point out some elementary properties of these equations. Next we state some theorems first proved in Ref. 1 for the nonexistence of solutions to Eqs. (1) and (2) in a zero gravitational field. If the curvature of the perimeter of the domain is sufficiently large at a point, then there exists a critical contact angle such that Eqs. (1) and (2) have no solution for $\gamma < \gamma_{\text{crit}}$. We give the value of γ_{crit} for a sharp corner and a lower bound on γ_{crit} for a rounded corner. We then describe the nature of the solutions in a nonzero gravitational field.

Next we describe JASON, a general purpose computer program that solves second-order elliptic partial differential equations in two dimensions on a nonuniform quadrilateral mesh by a finite element method. JASON is reliable and easy to use, but it is not necessarily the most efficient program for this problem, since it is designed for a very general class of problems.

We consider the system of discrete equations corresponding to Eqs. (1) and (2) for a particular mesh. We study how the number of iterations and computer time required to solve the discrete equations depend on the mesh spacing for uniform meshes. Next we explore how the accuracy of the computed solution varies over the cross section with the mesh spacing

and with the contact angle, on a square cross section for the case of zero gravity. A closed-form solution to Eqs. (1) and (2) is known for this case.

Next we calculate capillary surfaces on elliptical cross sections. We investigate how the height at various points on the cross section depends on the contact angle and the ratio of the major and minor axes. Numerical estimates of γ_{crit} are obtained and compared with the lower bounds mathematically derived from a theorem given in Ref. 1.

We describe a procedure for calculating capillary surfaces on cross sections with sharp corners for values of γ less than γ_{crit} . We use this method to calculate surfaces on a square cross section and on a circular cross section with a reentrant notch. Finally, we discuss how the height of the surface at various points on these cross sections depends on the contact angle.

2. DEFINITION OF THE PROBLEM

We consider the equilibrium free surface of a liquid partly filling a vertical cylinder for the case in which the surface height $u(x,y)$ is a single-valued smooth function of x and y and in which there is sufficient liquid to cover the base of the cylinder entirely. The gravitational field is taken to be positive when directed vertically downward. The height then satisfies the equation

$$\begin{aligned} \nabla \cdot \left(\frac{1}{W} \nabla u \right) &= \kappa u + 2H \\ W &= (1 + |\nabla u|^2)^{\frac{1}{2}}, \end{aligned} \tag{1}$$

where ∇ is the two-dimensional operator $(\partial/\partial x, \partial/\partial y)$, $\kappa = \rho g/\sigma$ is the capillary constant, ρ is the difference in densities between the liquid and gas phases, g is the acceleration due to gravity, and σ is the gas-liquid surface tension. The constant $2H$ is determined by the cross-sectional shape of the cylinder, the volume of the liquid, and the boundary condition satisfied by the free surface of the liquid at the cylinder wall.

The boundary conditions for a free surface that makes a contact angle γ with the cylinder wall is

$$\frac{1}{W} \frac{\partial u}{\partial n} = \cos \gamma \quad \text{at the wall,} \quad (2)$$

where $\partial u/\partial n$ denotes the derivative of u with respect to the outward directed normal at the wall. Only the case of wetting liquids, $0^\circ \leq \gamma < 90^\circ$, will be considered here. (The nonwetting case can be obtained from it directly by means of a simple transformation.)

3. ELEMENTARY PROPERTIES

The quantity $\nabla \cdot (W^{-1} \nabla u)$ in Eq. (1) is twice the mean curvature of the surface $z = u(x, y)$. Thus in a zero-gravity field ($\kappa = 0$) the free surface has constant mean curvature.

If one integrates Eq. (1) over the cross section of the cylinder, and uses Eq. (2), one obtains

$$\kappa A \bar{u} + 2HA = L \cos \gamma, \quad (3)$$

where $\bar{u} = A^{-1} \int_{\Omega} u \, dx \, dy$ is the average height of the free surface, and A and L are the area and perimeter, respectively, of the cross section Ω .

For the case $\kappa \neq 0$, if $u(x,y)$ is a solution of Eqs. (1) and (2) for one value of H , then $u(x,y)$ plus a constant is a solution for any other value of H . The solution is unique for a particular value of H if $\kappa \geq 0$. The value of H is related to the reference level from which the height of the capillary surface is measured. It is sometimes convenient to measure the height of the surface from the level of an infinite reservoir into which the cylinder, without bottom, is dipped. On the surface of the reservoir, infinitely far from the cylinder, $u=0$, $\nabla u=0$, and therefore $H=0$. The average height $\bar{u}_0$ to which the capillary surface inside the cylinder rises above the reservoir is then obtained from Eq. (3).

$$\bar{u}_0 = (L \cos \gamma) / \kappa A .$$

For the case $\kappa = 0$, one cannot arbitrarily choose H . It is determined by Eq. (3).

$$2H = (L \cos \gamma) / A . \quad (3)$$

For $\kappa = 0$, the solution of Eqs. (1) and (2) is determined only up to an additive constant. A convenient way to choose this constant is to take $u=0$ at the lowest point of the capillary surface. For uniformity all the numerical results presented in this report will use this choice for $u=0$, both for the case $\kappa = 0$ and for $\kappa \neq 0$. This will enable us to compare directly calculations for different values of κ .

4. NONEXISTENCE OF SOLUTIONS FOR THE CASE $\kappa = 0$

For each cylinder, there may exist a critical contact angle such that Eqs. (1) and (2) have no solution for $0 \leq \gamma < \gamma_{\text{crit}}$. Several important theorems have been formulated in Refs. 1,4 that relate γ_{crit} to the shape of the cross section of the cylinder. We give below forms of them relevant to our problem.

Theorem 1. Let the cross-section boundary have a corner with an interior angle 2α . Then a solution of Eqs. (1) and (2) can exist in the neighborhood of that corner only if

$$\gamma \geq 90^\circ - \alpha$$

and no solution exists if

$$\gamma < 90^\circ - \alpha.$$

Example: $\alpha = 45^\circ$ for a square cross section; thus the critical contact angle is $\gamma_{\text{crit}} = 45^\circ$. There is no solution for $0 \leq \gamma < \gamma_{\text{crit}}$.

A similar result holds for a region on a curved boundary on which the curvature is large relative to a value determined by the entire cross section.

Theorem 2. Suppose there is a point p on the boundary at which the curvature is greater than L/A ; then there exists a critical contact angle such that there is no solution of Eqs. (1) and (2) in a neighborhood of p for $0 \leq \gamma < \gamma_{\text{crit}}$.

Example: Let the cross section be an ellipse. The curvature of an ellipse is greatest at the point where the semimajor axis cuts the boundary. The curvature at this point exceeds L/A when the ratio b of semiminor

and semimajor axes is less than 0.6116. According to Theorem 2, there exists a critical contact angle for an ellipse with $b < 0.6116$ [2].

A third theorem gives a lower bound for γ_{crit} . Consider the cross section of a cylinder shown in Fig. 1. Let A be the area of the entire cross section, and L be its perimeter. Let the cross section be cut by a curve Γ , which intersects the perimeter at points p_1 and p_2 . The curve Γ divides the area of the cross section into two parts, A^* and $A - A^*$, and divides the perimeter into two parts, L^* and $L - L^*$. Let $|\Gamma|$ denote the length of the curve Γ from p_1 to p_2 . Then the following theorem holds [1].

Theorem 3. Let V be the function

$$V = \frac{|\Gamma|A}{|L^*A - A^*L|} ; \quad (4)$$

then

$$\cos \gamma_{\text{crit}} \leq V_0 ,$$

where V_0 is the minimum of V with respect to all possible curves Γ .

This minimization can be done in two steps. First, find the Γ that minimizes V for a fixed pair of intersection points, p_1 and p_2 ; then vary p_1 and p_2 .

For any p_1 and p_2 , the Γ that minimizes V is an arc of a circle with radius

$$R = \frac{A}{LV_p(p_1, p_2)} , \quad (5)$$

where $V_p(p_1, p_2)$ is the minimum of V for fixed p_1 and p_2 [2].

solution of Eqs. (4) and (5) gives $V_p(p_1, p_2)$. Finally, minimization of $V_p(p_1, p_2)$ with respect to p_1 and p_2 gives V_0 .

Example: The lower bounds for γ_{crit} for ellipses with ratio b of semiminor and semimajor axes are:

b	Bound
0.20	35.12°
0.25	26.95°
0.33	16.88°
0.40	10.32°
0.50	3.71°
0.60	0.12°

Numerical solution of Eqs. (1) and (2) indicates that these bounds are close to γ_{crit} .

5. BEHAVIOR OF SOLUTIONS FOR THE CASE $\kappa \neq 0$

For the case $\kappa \neq 0$, Eqs. (1) and (2) have a solution for each γ . However, the behavior of the solution is different for $\gamma < \gamma_{\text{crit}}$ and $\gamma \geq \gamma_{\text{crit}}$ [3].

Theorem 4. Let the cross-section boundary have a corner with an interior angle 2α . Let ρ and θ be polar coordinates centered at the corner with θ measured from the bisector of the corner angle. Let

$$q = \frac{\cos \gamma}{\sin \alpha} = \frac{\cos \gamma}{\cos \gamma_{\text{crit}}},$$

where $\gamma_{\text{crit}} = 90^\circ - \alpha$, as in the case $\kappa = 0$. If $\gamma \geq \gamma_{\text{crit}}$, then $u(\rho, \theta)$ is bounded in the neighborhood of the corner.

If $0 \leq \gamma < \gamma_{\text{crit}}$, then $u(\rho, \theta)$ is asymptotic to

$$u(\rho, \theta) \sim u_0(\rho, \theta) + [q \cos \theta - (1 - q^2 \sin^2 \theta)^{\frac{1}{2}}] / \kappa \rho \quad (6).$$

as $\rho \rightarrow 0$, where u_0 is $O(1)$. Inside the cylinder u grows like $1/\rho$ as the corner is approached.

The solution in a cylinder with a curved boundary is bounded for all γ . However, this bound depends inversely on the radius of the corner [4].

Theorem 5. Let C be the maximum curvature of the cross-section boundary, and let $r = 1/C$. Then in a neighborhood of the corner

$$u(x, y) < r + \frac{2}{\kappa r} \quad (7)$$

6. JASON

The computer program JASON solves the nonlinear elliptic partial differential equation in two independent variables [5]:

$$\nabla \cdot (c \nabla \phi) = a \phi + b \quad (8)$$

with boundary condition:

$$c \nabla \phi \cdot \hat{n} = f \phi + g \quad , \quad (9)$$

where $a = a(x, y)$, $b = b(x, y)$, $c = c(x, y, |\nabla \phi|^2)$, $f = f(s)$, $g = g(s)$, and s is the arc length along the boundary. It uses a bilinear finite element method on a nonuniform quadrilateral mesh. The resulting algebraic system of equations is solved by the one-step block successive over-relaxation-Newton method (BSOR-Newton).

The domain of a problem suitable for JASON can be composed of one or more distinct subregions separated by common boundaries. Each subregion

can have different functions a , b , and c . If the values of a , b , and c for a particular subregion are constant, they can be specified on a data card; if they are functions of x , y , or $|\nabla\phi|^2$, JASON must be supplied with a subroutine to calculate them. One can suppress solution of Eq. (8) in a particular subregion by specifying $c=0$ in that subregion.

JASON contains a mesh generator that produces a smooth mesh by "equipotential zoning." Input to the mesh generator consists of the set of boundary points of each subregion. Each point is specified by four numbers: the x and y coordinates of the point, and the (integer) L and M values of mesh line coordinates through the point. One need not specify every boundary point. JASON will compute by linear interpolation the boundary points that have been skipped, if they lie on the same mesh line.

Dirichlet boundary conditions can be imposed at any point in the mesh. Neumann boundary conditions are restricted to the boundary of the entire domain of the problem and the boundaries between subregions with $c=0$ and those with $c \neq 0$.

Before using JASON, one should make a rough sketch of the desired mesh, to guide the choice of the boundary points. These define a polygon whose boundary approximates that of the original domain. For the case $\kappa=0$, one must calculate the perimeter and area of this polygon, in order to calculate H .

The input to JASON is a series of data cards. The first card specifies the procedures to be performed: generate a mesh, plot the mesh, solve Eq. (8) for ϕ , calculate $\nabla\phi$, and plot ϕ . The second card is the title for printed and plotted output. The third card gives

the size of the mesh for the entire domain, L_{MAX} and M_{MAX} . The mesh coordinates take the values $1 \leq L \leq L_{MAX}$ and $1 \leq M \leq M_{MAX}$.

The next input is a set of cards for each subregion. The first card of each set lists the values of a , b , and c for a subregion, or provides parameters for a subroutine that calculates a , b , and c . The remaining cards of the set give the boundary points of that subregion.

The next cards contain the values of L , M , f , and g at enough points to specify the boundary conditions. If f and g are constant along a boundary, one needs to give only L , M , f , and g at the first boundary point and L and M at the subsequent corners of that boundary.

The next card allows one to choose the iteration control parameters of the solution subroutines. The remaining cards specify the domains for which the values of ϕ or $\nabla\phi$ are to be printed or the domain in which ϕ is to be plotted.

7. SQUARE CROSS SECTION WITH $\kappa=0$ AND $\gamma \geq \gamma_{crit}$

The convergence properties of JASON were studied by calculating the capillary surfaces for $\kappa=0$ in a cylinder with a square cross section. The exact solution is known for $45^\circ \leq \gamma \leq 90^\circ$ and is a portion of a lower hemisphere. The square had an edge of length 2 and was centered at the origin. It was the domain $-1 \leq x \leq 1$ and $-1 \leq y \leq 1$. Figure 2 shows the height of the capillary surface along the edge of the square $x=1$ for contact angles $\gamma=45^\circ$, 50° , 55° , and 60° . For $\gamma=\gamma_{crit}=45^\circ$, the slope is infinite at the corner $x=1$ and $y=1$, although the rise height is finite.

The same data are graphed in a different way in Fig. 3. This figure shows how the height at several fixed points on the edge of the square varies with the contact angle γ . For $\gamma = 90^\circ$ the surface is flat. Figure 3 shows that the height in the corner increases rapidly as γ nears γ_{crit} . The height at other points on the edge varies much less rapidly with γ .

The coordinate axes $x=0$ and $y=0$ are lines of reflection symmetry, so the solution in one quadrant repeats in the other three quadrants. The solution was calculated in the first quadrant, $0 \leq x \leq 1$ and $0 \leq y \leq 1$. The boundary conditions are: $\hat{n} \cdot \nabla u = 0$ on the lines $y=0$ and $x=0$, and $(\hat{n} \cdot \nabla u)/W = \cos \gamma$ on the lines $x=1$ and $y=1$. Here $\hat{n}$ denotes the outward directed unit normal for each edge.

Capillary surfaces were calculated on uniform meshes with mesh spacing $h = 0.2, 0.1$, and 0.05 . Surfaces were calculated for contact angle $\gamma = 45^\circ, 50^\circ, 55^\circ$, and 60° for each mesh spacing.

Surfaces were also calculated using two nonuniform meshes, which were successive refinements of the uniform mesh with $h=0.05$. The refinements were made near the corner of the square. The first mesh (NU1) had $h=0.05$ for $0 \leq x \leq 0.8$ or $0 \leq y \leq 0.8$ and $h=0.025$ for $0.8 \leq x \leq 1.0$ or $0.8 \leq y \leq 1.0$. The second mesh (NU2) was a refinement of NU1 which had $h=0.0125$ for $0.9 \leq x \leq 1.0$ or $0.9 \leq y \leq 1.0$.

We now consider the number of relaxation cycles required to solve the system of discrete equations for a particular mesh. In subsequent paragraphs we will discuss how the solution of the discrete equations approaches the solution of Eqs. (1) and (2) as the mesh is refined.

The number of cycles required to solve the system of discrete equations depends on the mesh spacing. This was studied by calculating the surfaces for $\gamma = 50^\circ$ on a sequence of uniform meshes. Each mesh had n equally spaced horizontal mesh lines and n vertical mesh lines. The meshes were 6×6 , 11×11 , 16×16 , and 21×21 . JASON solves the discrete equations by the one-step block successive over-relaxation-Newton method, BSOR-Newton [6].

These results are compared with those of another program, which solves the discrete equations by a dynamic alternating direction implicit method, DADI [7]. Both computations were performed on a CDC 7600. The number of cycles and CPU-seconds required are shown in Table 1.

TABLE 1. Comparison of BSOR-Newton with DADI
on a square domain with n vertical and
 n horizontal mesh lines.

Method	Final R/L		$n = 6$	$n = 11$	$n = 16$	$n = 21$
BSOR-Newton	1×10^{-6}	Cycles used:	22	36	63	84
BSOR-Newton	1×10^{-6}	CPU-sec used:	0.615	3.660	13.152	30.018
DADI	1×10^{-8}	Cycles used:	12	16	18	24
DADI	1×10^{-8}	CPU-sec used:	0.023	0.088	0.204	0.465

The DADI method is approximately 18 times faster per cycle than JASON. However, JASON is a general-purpose program that solves the discrete equations on a nonuniform quadrilateral mesh, and would be expected to be slower than the DADI program, which was written specifically for a uniform rectangular mesh for this problem. JASON is reliable and easy to use, but is not necessarily efficient for this problem.

The number of cycles required for JASON to solve the discrete equations depends on the criterion for terminating the iteration and the procedure followed in optimizing the relaxation parameter ω . The termination criterion used here is that $R/L < 1 \times 10^{-6}$. R is the square root of the sum of the squares of the residual at each point. L is the square root of the sum of the squares at u at each point.

The initial value of ω is 1.5. This was used until R/L was less than 1×10^{-2} , then ω was adjusted upward toward the estimated asymptotically optimal value, half the estimated increment every five SOR iterations.

The number of cycles required depends on these iterations parameters. However, Table 1 gives a rough measure of the amount of computing necessary to solve the discrete equations, and how this depends on the mesh spacing.

The number of cycles required to solve the discrete equations depends only weakly on the contact angle γ . This can be seen by comparing the values of R/L for different γ after the same number of relaxation cycles. On a 21×21 uniform mesh, 80 cycles reduced R/L to 2.9×10^{-6} for $\gamma = 45^\circ$ and 2.1×10^{-6} for $\gamma = 60^\circ$. On an 11×11 uniform mesh, 30 cycles reduced R/L to 15.0×10^{-6} for $\gamma = 45^\circ$ and 8.7×10^{-6} for $\gamma = 60^\circ$. This weak dependence on γ is shown in more detail in Table 2.

Table 2. $R/L \times 10^{-6}$ after n cycles for various γ .

Mesh	Cycles	$\gamma = 45^\circ$	$\gamma = 50^\circ$	$\gamma = 55^\circ$	$\gamma = 60^\circ$
11x11	30	15.0	12.5	10.3	8.7
21x21	80	2.9	2.6	2.3	2.1

Table 3 shows an experimental study of the convergence of the solution of the discrete equations toward the known solution of Eqs. (1) and (2) as the mesh spacing decreases. The tabulated quantity δu is the difference between the known solution and the solution computed with a particular mesh. It is tabulated as a function of contact angle γ , mesh spacing h , and position y along the edge of the square. The point $y=1$ is the corner, and $y=0$ is the midpoint of the full square.

Table 3 shows that for fixed values of γ and h , δu is larger for y near the corner. It further shows that for fixed values of y and h , δu is larger for γ near 45° .

In the remaining paragraphs, we shall discuss how δu changes with h for fixed values of γ and y . We consider first the uniform meshes. Table 3 shows that for $0 \leq y \leq 0.9$, δu decreased by $1/4$ when h was decreased by $1/2$. That is, δu is proportional to h^2 for these values of y on uniform meshes. However, δu decreased less rapidly than h^2 at the corner $y=1$. Convergence is poorer at the corner probably because the slope is very large there.

We consider next the nonuniform meshes. The mesh NU1 has $h=0.05$ for $0 \leq y \leq 0.8$ and $h=0.025$ for $0.8 \leq y \leq 1.0$. We shall compare the δu on NU1 with that on the uniform mesh with $h=0.05$. For both the 45° and 50° cases, δu decreased for $0.9 \leq y \leq 1.0$, δu was about the same for $y=0.85$, δu increased for $y=0.8$, and δu was about the same for $0 \leq y \leq 0.6$. That is, δu decreased in the upper half of the refined region, increased at the boundary of the refined and unrefined regions, and was about the same in the interior of the unrefined region.

The mesh NU2 has $h=0.0125$ for $0.9 \leq y \leq 1.0$ and has h the

TABLE 3. $\delta u \times 10^5$ for $x=1.0$ and $0 \leq y \leq 1.0$.

h	y = 1.0	0.95	0.9	0.85	0.8	0.6	0.4	0.2	0.0
$\gamma = 45^\circ$									
0.2	34166				2051	487	198	108	84
0.1	26689		2114		473	102	46	26	20
0.05	20944	2239	515	161	77	25	12	7	5
NU1	16761	832	220	172	140	33	11	6	2
NU2	13478	434	291	217	194	29	6	3	2
$\gamma = 50^\circ$									
0.2	4186				831	295	143	86	70
0.1	1804		503		209	73	35	21	17
0.05	701	258	125	75	51	19	9	5	5
NU1	304	117	81	71	64	20	8	5	4
$\gamma = 55^\circ$									
0.2	1468				391	173	94	60	50
0.1	529		188		101	44	23	14	12
0.05	176	78	48	33	26	11	6	4	3
$\gamma = 60^\circ$									
0.2	605				192	97	57	39	33
0.1	199		82		50	25	14	10	8
0.05	62	31	21	16	13	6	4	3	2

same as NU1 for other values of y . We shall compare the δu on NU2 with that on NU1. It decreased for $0.95 \leq y \leq 1.0$, increased for $0.8 \leq y \leq 0.9$, and was about the same for $0 \leq y \leq 0.6$. That is, δu decreased in the upper half of the refined region, increased in the region of intermediate mesh spacing, and was about the same in the region with $h = 0.05$.

8. ELLIPTICAL CROSS SECTION

Capillary surfaces were calculated for cylinders of elliptical cross section with semimajor axis $a = 1.0$ and semiminor axes $b = 0.60, 0.33$, and 0.20 . The cases $b = 0.60$ and 0.33 were calculated for $\kappa = 0$. The case $b = 0.20$ was calculated for both $\kappa = 0$ and $\kappa = 1$. Closed form solutions are not known for the ellipse as they are for the square for $\kappa = 0$.

Figure 4 shows how a quadrilateral mesh was fit to $1/4$ of an ellipse. The $1/4$ ellipse was made into a four "sided" figure by choosing a point on the curved edge and using it as a fourth corner. A mesh was fit to this by taking one pair of opposite sides to be mesh lines with constant mesh coordinate L , and the other pair to be mesh lines with constant coordinate M .

Figures 5 and 6 show the 11×6 meshes generated for the cases $b = 0.33$ and 0.20 . Figure 7 shows the 21×11 mesh generated for $b = 0.20$. Figure 8 shows the level curves of the capillary surface for the case $b = 0.33$ and $\gamma = 60^\circ$.

According to Theorem 2 there will be a critical contact angle if

the curvature at any point on the ellipse exceeds the ratio of its perimeter to its area. This occurs if $b/a < 0.6116$. Theorem 3 gives a lower bound for the critical angle. These are shown in Table 4. For the case $\kappa = 0$, capillary surfaces exist for $\gamma \geq \gamma_{\text{crit}}$, but not for $\gamma < \gamma_{\text{crit}}$. For $\kappa \neq 0$, capillary surfaces exist and are bounded for $\gamma < \gamma_{\text{crit}}$, but the bound is inversely related to both κ and the maximum radius of curvature of the ellipse, as in Eq. (7).

Theorems 2 and 3 restrict the existence of capillary surfaces for a cross section with a smoothly curved boundary. However, the actual cross section that is used is not an ellipse, but a polygonal approximation to an ellipse. Because of this, Theorem 1 gives an additional existence criterion, which depends on the interior angles at the polygon's corners. By Theorem 1 the critical angle is $\gamma_{\text{crit}} = 90^\circ - \alpha$, where 2α is the smallest interior angle. The γ_{crit} from Theorem 1 are shown in Table 4.

Theorems 1, 2, and 3 limit the existence of solutions of the differential Eqs. (1) and (2). However, the discrete system of equations approximating (1) and (2) can have a solution even when Eqs. (1) and (2) do not. This is worth remembering because the 11×6 meshes used to explore the ellipse problem are rather coarse, especially for the largest ellipse, $b = 0.60$. Thus the local truncation error, which is of the order of the mesh spacing squared, is not very small.

The computing times used to calculate the various capillary surfaces are shown in Table 5. For the $\kappa = 0$ cases, the smallest time was for the largest contact angle. For example, for the $b = 0.60$ case, with the 11×6 mesh, 1.13 CPU seconds were used to calculate the surface for $\gamma = 40^\circ$, and 1.57 CPU seconds were used for $\gamma = 0^\circ$. However, for the $\kappa = 1$ case, the smallest time was for the smallest γ . Note that it took approximately

TABLE 4. γ_{crit} from Theorems 1 and 2 for various meshes and values of b .

b	Mesh	γ_{crit}	
		Theorem 3	Theorem 1
0.60	11×6	$\geq 0.12^\circ$	8.79°
0.60	21×11	$\geq 0.12^\circ$	4.55°
0.33	11×6	$\geq 16.88^\circ$	15.71°
0.20	11×6	$\geq 35.12^\circ$	24.89°
0.20	21×11	$\geq 35.12^\circ$	13.43°

TABLE 5. CPU-sec used for various meshes and values of b .

b	κ	Mesh	CPU - sec
0.60	0	11×6	1.13 - 1.57
0.60	0	21×11	19.23 - 19.39
0.33	0	11×6	3.66 - 6.24
0.20	0	11×6	6.20 - 11.60
0.20	0	21×11	44.70 - 71.57
0.20	1	11×6	7.71 - 9.38

the same time to compute surfaces for the ellipse with its irregular mesh as for the rectangle with its regular mesh. The rectangle with 64 mesh points took 1.22 CPU seconds. The ellipse with the 11×6 mesh took 1.13–1.57 CPU seconds for the $b = 0.60$ case. The $b = 0.33$ and 0.20 cases took more time, but these surfaces had steep gradients.

The computing time depends on the iteration control parameters. Because the 11×6 mesh is rather coarse, $R/L < 1.0 \times 10^{-4}$ was used in most calculations for the criterion for terminating the iteration. For the 21×11 mesh a stronger criterion was used, $R/L < 1.0 \times 10^{-5}$. The default value that JASON assumes is 1.0×10^{-6} .

Three iteration parameters can be chosen to attempt the minimization of the computing time. They are: the initial value of ω , the value of R/L at which one begins to adjust ω towards its estimated optimal value, and the fraction of the distance moved toward this value. The default values of these parameters are 1.5, 1.0×10^{-3} , and 0.06. However, it was found that for most of the capillary surface calculations, JASON can solve the discrete system of equations if the values 1.5, 1.0×10^{-2} , and 0.60 are used. Computing time is less with these values because fewer steps are used before changing ω and optimization is pursued more vigorously.

JASON prints the values of R/L and other quantities at every tenth iteration. If the solution attempt fails, one can examine this sequence of values and decide how to change the iteration control parameters. If R/L increases during the cycles when the initial ω is being used, then the initial ω should be reduced, say to 1.2. If R/L decreases while the initial ω is being used, but increases after optimization begins,

the fraction for the ω optimizer should be reduced. If this does not succeed, it may be necessary to reduce the value of R/L at which optimization begins.

Figure 9 shows the height of the capillary surfaces at the point A where the semimajor axis intersects the cylinder wall. Figure 10 shows the height at the point B where the semiminor axis intersects the cylinder wall. The height is taken to be zero at the center of the elliptical cross section. Figures 9 and 10 show $u(A)$ and $u(B)$ as a function of the contact angle γ for the four cases: $b=0.20$, 0.33 and 0.60 each with $\kappa=0$, and $b=0.20$ with $\kappa=1$. Figure 9 shows that for fixed γ , $u(A)$ is larger for smaller values of the semiminor axis b , while Fig. 10 shows that for fixed γ , $u(B)$ is larger for larger values of b .

We shall discuss first the case $b=0.20$ with $\kappa=0$. In this case the effect of the curvature of the actual ellipse near its major axis can be distinguished from the effect of the corner at point A of the polygonal approximation to the ellipse. The corner by itself would cause a γ_{crit} of 24.89° for the 11×6 mesh and one of 13.43° for the 21×11 mesh. However, the ellipse's curvature overwhelms this effect and causes a $\gamma_{\text{crit}} \geq 35.12^\circ$. Figure 9 shows that $u(A)$ becomes large with increasing rapidity as γ approaches 35° . Furthermore, when the mesh is refined from 11×6 to 21×11 ; the value of $u(A)$ at 35° increases by 12%, while that at 40° increases by less than 1%. This must be the effect of the ellipse's curvature, since the effect of the approximating polygon's corner is reduced for the refined mesh. This indicates that the γ_{crit} due to the ellipse's curvature is near 35° , and that the lower bound given by

Theorem 3 is indeed close to γ_{crit} .

Consider next the case $b=0.20$ with $\kappa=1$. The capillary surface for a smooth ellipse is bounded at A because it has finite curvature. However, $u(A)$ should become infinite for γ less than the γ_{crit} of the approximating polygon's corner. Figure 9 shows that $u(A)$ for the 11×6 mesh becomes larger as γ approaches 25° , as is expected. Although the values of $u(A)$ are quite different for the cases $\kappa=0$ and $\kappa=1$, the values of $u(B)$ are almost the same. At 35° they differ by only 0.3%.

For the case $b=0.33$ with $\kappa=0$, the effects of the ellipse's curvature and the approximating polygon's corner cannot be distinguished for the 11×6 mesh. The first predicts a $\gamma_{\text{crit}} \geq 16.88^\circ$ and the second a $\gamma_{\text{crit}} = 15.71^\circ$. Figure 9 shows that $u(A)$ and $|du(A)/d\gamma|$ become large as γ approaches 15° , which is consistent with these predictions. It also shows that the γ_{crit} due to the ellipse's curvature cannot be much larger than 16.88° . This illustrates that the lower bound given by Theorem 3 is again close to γ_{crit} .

Finally, for the case $b=0.60$ with $\kappa=0$, the coarseness of the mesh caused the solution of the discrete system of equations to differ somewhat from those for the cases $b=0.20$ and 0.33 . The sharp corner should give a γ_{crit} of 8.79° for the 11×6 mesh and 4.55° for the 21×11 mesh. The lower bound on γ_{crit} due to the ellipse's curvature is 0.12° . However, Fig. 9 shows that although $u(A)$ increases as γ approaches 0° , $|du(A)/d\gamma|$ decreases. When the mesh was refined from 11×6 to 21×11 , $u(A)$ increased by 9%, 7%, 4%, and 2%, at $\gamma=0^\circ$, 5° , 10° , and 15° , respectively. The relatively larger increase for 0° and 5° than for 15° shows the effects of the corner, but not as dramatically as for the $b=0.20$ case. The coarseness of the mesh is shown by the change in $u(B)$ when the

mesh was refined. It changed by 6%, 5%, 4%, and 3%, at $\gamma = 0^\circ, 5^\circ, 10^\circ$, and 15° , respectively. In contrast, for the case $b = 0.20$ with $\kappa = 0$, $u(B)$ changed by only 0.6% when the mesh was refined.

9. CALCULATING CAPILLARY SURFACES ON CROSS SECTIONS WITH CORNERS

A cylinder whose cross section has a corner, as in Fig. 11A, will have a critical contact angle. If the interior angle at the corner is 2α , then $\gamma_{\text{crit}} = 90^\circ - \alpha$. There are no solutions to Eqs. (1) and (2) for $\kappa = 0$ and $\gamma < \gamma_{\text{crit}}$. Solutions exist for $\kappa \neq 0$ and $\gamma < \gamma_{\text{crit}}$, but the height goes to infinity at the corner. It would be difficult to compute such a surface numerically over the entire cross section. Instead, the cross section is divided into two regions, as with curve AA' of Fig. 11A. One is a small region Ω_c that includes the corner; the other Ω_r is the remainder of the cross section. The asymptotic form of the surface near the corner region is known. The surface on the remainder Ω_r can be calculated numerically, with the boundary condition that it match the asymptotic solution along the curve AA' .

The boundary data are the values of the function $(\hat{n} \cdot \nabla u)/W$ at each point on the boundary. W is the function $(1 + |\nabla u|^2)^{1/2}$, and $\hat{n}$ is the outward directed normal at the boundary. $(\hat{n} \cdot \nabla u)/W$ is $\cos \gamma$ at the cylinder wall. It is zero on boundaries that are lines of reflection symmetry. It is matched with that of the asymptotic solution along the boundary curve AA' .

The surface in a neighborhood of the corner has the asymptotic form [3]

$$u(\rho, \theta) \sim u_0(\rho, \theta) + v(\rho, \theta) \quad . \quad (10)$$

where u_0 is a function of $O(1)$ and

$$v(\rho, \theta) = \frac{1}{\kappa \rho} [q \cos \gamma - (1 - q^2 \sin^2 \theta)^{1/2}] . \quad (11)$$

The quantities ρ and θ are polar coordinates of a point on the cross section; ρ is the radial distance from the corner, and θ is the angle measured from the bisector of the corner angle. These are shown in Fig.

11B. The quantity q is

$$q = \frac{\cos \gamma}{\sin \alpha} = \frac{\cos \gamma}{\cos \gamma_{\text{crit}}} \quad (12)$$

For $\rho \ll 1$, we have $u_0 \ll v$.

The boundary condition function $(\hat{n} \cdot \nabla u)/W$ can be broken into two factors, a magnitude and the inner product of two unit vectors.

$$\frac{\hat{n} \cdot \nabla u}{W} = \frac{|\nabla u|}{W} \frac{\hat{n} \cdot \nabla u}{|\nabla u|} . \quad (13)$$

We do not know the order of ∇u_0 , but we know that $|\nabla v|$ is $O(1/\rho^2)$, so that in general $|\nabla u|$ also must be at least $O(1/\rho^2)$. Consequently,

$$\begin{aligned} \frac{|\nabla u|}{W} &= 1 - \frac{1}{2|\nabla u|^2} + \dots \\ &= 1 - O(\rho^4) . \end{aligned} \quad (14)$$

Thus if the curve AA' is sufficiently near the corner, then $|\nabla u|/W$ is approximately 1.

We next consider the factor $(\hat{n} \cdot \nabla u)/|\nabla u|$. The quantity $\nabla u/|\nabla u|$ is a unit vector normal to a level curve of u . If we choose the curve AA' to be this level curve, then $\hat{n} = \nabla u/|\nabla u|$, and so $(\hat{n} \cdot \nabla u)/|\nabla u|$ will be 1. The level curve of u is not known, but for small ρ we have $u_0 \ll v$, so a level curve of u is approximately a level curve of v . We shall

choose the curve AA' to be a level curve of v ; thus the factor $(\hat{n} \cdot \nabla u)/|\nabla u|$ will be approximately 1.

The level curves of v are a family of circles, which depend on the contact angle γ . The radius of a circle is $1/\kappa v$, and its center lies on the bisector of the corner at a distance $q/\kappa v$ from the corner. The circle intersects the cross section of the cylinder wall at an angle γ , as shown in Fig. 11C.

Let u denote the solution of Eqs. (1) and (2) on the entire cross section with $(\hat{n} \cdot \nabla u)/W = \cos \gamma$ at the cylinder wall. Let u_r denote the solution of (1) and (2) on Ω_r with $(\hat{n} \cdot \nabla u)/W = \cos \gamma$ at the cylinder wall and with $(\hat{n} \cdot \nabla u)/W = 1$ on the curve AA' . It is shown in Ref. 8 that u_r is an upper bound to u at each point in Ω_r .

10. SQUARE CROSS SECTION WITH $\kappa=1$

The capillary surface over a square cross section was calculated for $\gamma=30^\circ$ and $\kappa=1$ by deleting the corner as described in the previous section. The value of γ_{crit} for a square is 45° . The calculation was performed on $1/4$ of a 2×2 square. The 9×9 mesh that was used is shown in Fig. 12. The boundary condition function $(\hat{n} \cdot \nabla u)/W$ is 0 along the reflection symmetry boundary BOB' . It is $\cos 30^\circ$ along the edges BA and $B'A'$, and is approximately 1 on the curve AA' that divides the corner from the remainder of the cross section. Curve AA' is composed of eight straight line segments, which approximate a level curve of v for $\gamma=30^\circ$.

The heights of the capillary surface along the edge AB and along

the diagonal CO are shown in Fig. 13. The height is taken to be zero at the center of the square, O . The height is approximately 1.80 on the boundary curve AA' and is almost constant along the curve. It differs by only 0.0062 between the endpoint A and the midpoint C of the curve.

The point B is the midpoint of the edge of the full square. The height of the capillary surface $u(B)$ is shown in Fig. 14 for $\kappa=1$ and $\gamma=30^\circ, 45^\circ, 50^\circ, 55^\circ$, and 60° . The four surfaces with $\gamma \geq \gamma_{\text{crit}}$ were calculated on a 6×6 mesh with uniform spacing. In the case $\kappa=0$, discussed previously, it was found that this mesh gives an accurate value for $u(B)$, although the height at the corner is inaccurate for $\gamma=45^\circ$. It is interesting to note that $u(B)$ changes almost uniformly over the range $30^\circ \leq \gamma \leq 90^\circ$. It does not change rapidly near $\gamma=45^\circ$ or in the range $30^\circ \leq \gamma \leq 45^\circ$. Although the fluid is drawn up to an infinite height in the corner, our calculation indicates that this does not affect dramatically the height at the midpoint.

11. CIRCULAR CROSS SECTION WITH A REENTRANT NOTCH

Capillary surfaces were calculated for a circular cross section with four rectangular reentrant notches as shown in Fig. 15A. The calculation was performed on $1/8$ of the cross section, which is shown in Fig. 15B. The circle has radius 1. The notch extends inward to a depth 0.2 on the axis and has half-width 0.2. The corner, point G of Fig. 15B, corresponds to a γ_{crit} of 50.77° .

A series of exploratory calculations were made with 9×8 meshes for $\kappa=1.0$ and $\gamma=0^\circ, 15^\circ, 30^\circ, 45^\circ$, and 60° . Figures 16 and 17 show the 9×8 meshes used for $\gamma=60^\circ$ and $\gamma=0^\circ$. The case $\kappa=1.0$ and $\gamma=0^\circ$

was calculated also with the 13×12 mesh shown in Fig. 18. The cases with $\gamma < \gamma_{\text{crit}}$ were calculated by deleting the corner as described previously.

The asymptotic solution of Eqs. (1) and (2) is not known for a corner which consists of a straight line intersecting a circular arc, as in Fig. 15C. However, the arc GHE differs only slightly from its chord GJE. The asymptotic solution for the corner which has CGJE for its cylinder wall is the function $v(\rho, \theta)$ defined previously. For our calculations, the dividing curve CDE was chosen to be a level curve of this $v(\rho, \theta)$.

Figures 19 and 20 show level curves of the numerical solutions for the 60° and 0° cases. In the 60° case, the fluid slopes gently up toward the cylinder wall and the corner G. In the 0° case, the fluid is drawn strongly up into corner G.

Figure 21 shows the variation of the height of the capillary surface with the contact angle γ , at various points on the cross section. The height is taken to be zero at the center of the circle, point O. The 13×12 and 9×8 meshes give somewhat different values for the surface height for $\gamma = 0^\circ$. The heights at points A, B, and F differ by the fractions $0.05/0.76$, $0.02/1.52$, and $0.07/1.42$. The meshes do not give high accuracy because only a few points are used to approximate the corner region, where the gradient is steep. However, these calculations show the general nature of the solution. Greater accuracy can be obtained by refining the mesh and moving the level curve CDE nearer the corner G.

Figure 22 shows the height of the surface for $\gamma = 60^\circ$ as a function of the arc length along the cylinder wall ABCGEF. It shows also the heights of the surfaces for $\gamma = 0^\circ$ and 30° along the wall from point A

to C and from E to F. The apparent discontinuity in the slope of the $\gamma = 0^\circ$ surface at point B results not from an actual discontinuity, but because the cylinder wall changes direction by 90° at B. The slopes on one side and the other of the point B in Fig. 22 refer to two different directions. For the 60° case, the fluid rises only slightly from 0.305 at F to 0.506 at corner G. In the 0° and 30° cases, it rises steeply as G is approached.

CDE is a level curve of v . It is a circular arc that intersects the cylinder wall at an angle γ . The curve CDE was approximated by 4 straight line segments of the 9×8 mesh and by 8 segments of the 13×12 mesh. Table 6 shows the calculated height along these level curves.

TABLE 6. Calculated height along CDE.

γ	Mesh	$u(C)$	$u(D)$	$u(E)$
0°	13×12	8.24	9.83	8.25
15°	9×8	5.36	5.76	5.16
30°	9×8	2.59	2.65	2.48
45°	9×8	0.930	0.933	0.913

The height is quite level along CDE for the 45° case. However, it increases by 16% at the middle of the curve for the 0° case. For this case, the level curve of u is less bowed toward the corner than the level curve of v . The level curves of u asymptotically approach circular arcs as their distance to the corner approaches zero, because u_0/v approaches 0. However, the point C is not very close to the corner. It is almost halfway from the corner G to point B. If a finer mesh is used, CDE can be chosen nearer the corner, where the level curve of v more closely approximates that of u .

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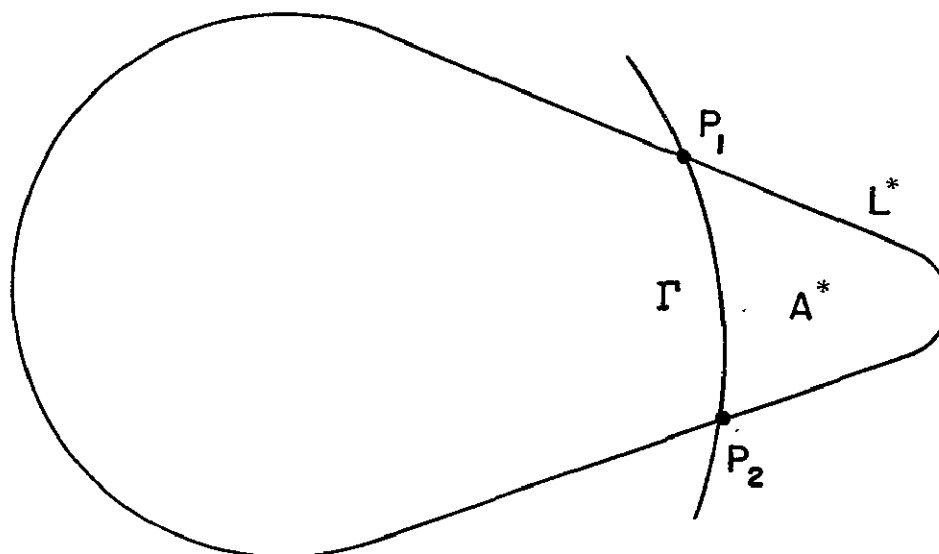
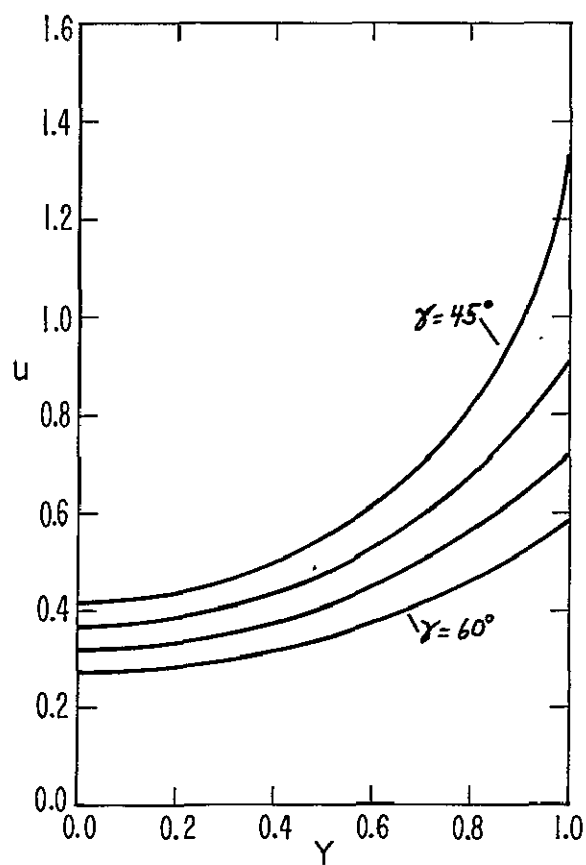


Fig. 1. Cross section of a cylinder.

(XBL 775-947)

Fig. 2. Height u of the capillary surface as a function of the distance y along the edge $x=1.0$ for $\kappa=0$ and $\gamma=45^\circ, 50^\circ, 55^\circ, \text{ and } 60^\circ$.

(XBL 776-1116)

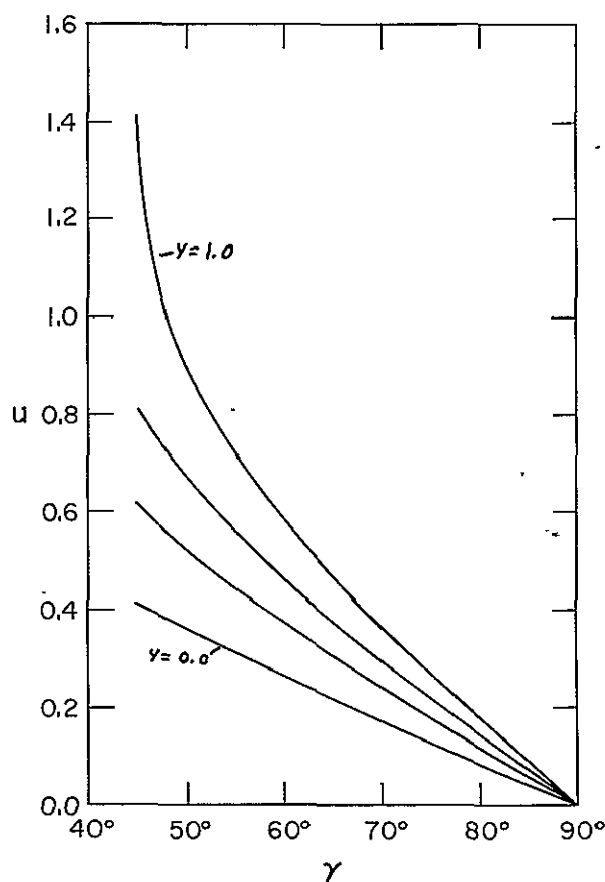


Fig. 3. Height u of the capillary surface as a function of the contact angle γ on the edge $x=1.0$ for $\kappa=0$ and $y=0.0, 0.6, 0.8$, and 1.0 . (XBL 775-954)

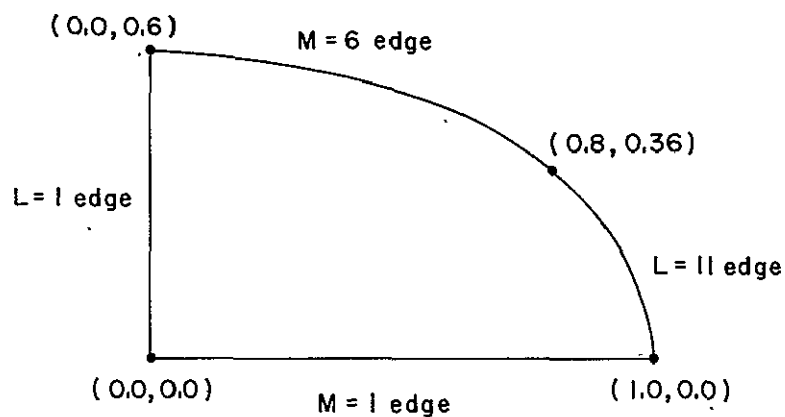


Fig. 4. One-fourth ellipse with $a=1.0$ and $b=0.6$ showing values of (x,y) at the corners and values of L or M on the edges. (XBL 775-948)

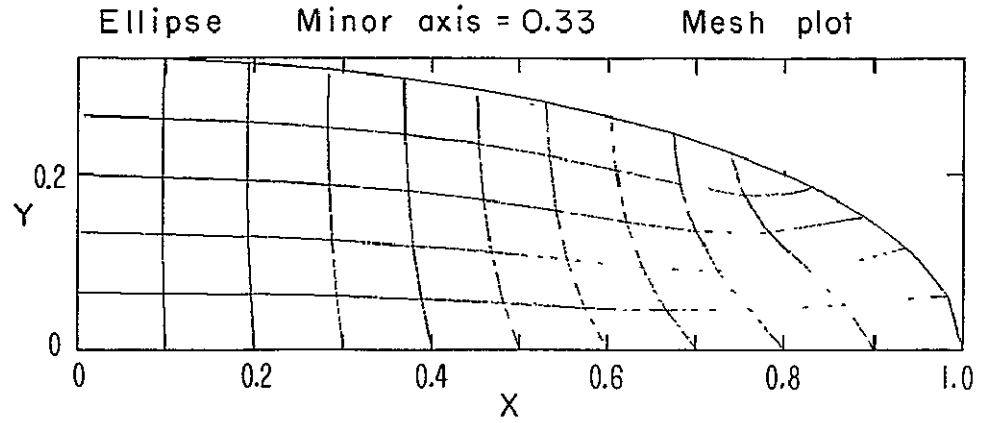


Fig. 5. 11×6 mesh for a 1/4 ellipse with $a=1.0$ and $b=0.33$. (XBL 776-1217)

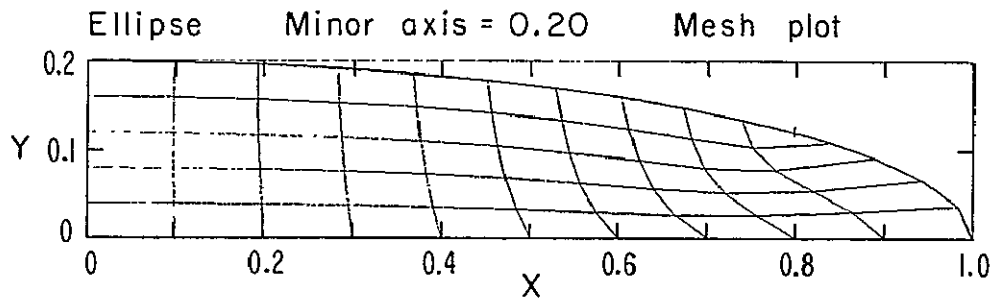


Fig. 6. 11×6 mesh for a 1/4 ellipse with $a=1.0$ and $b=0.20$. (XBL 776-1219)

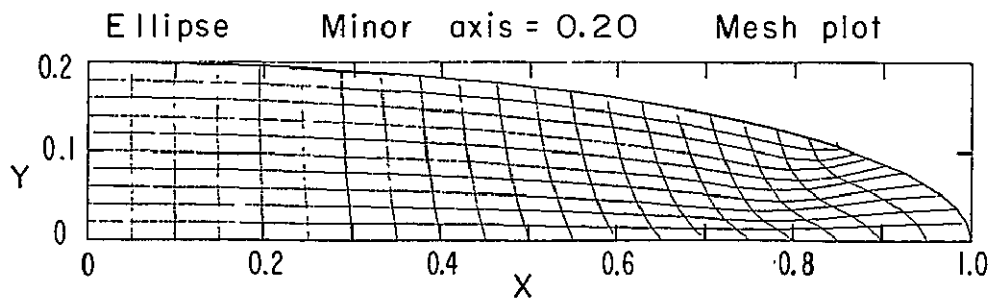


Fig. 7. 21×11 mesh for a 1/4 ellipse with $a=1.0$ and $b=0.20$. (XBL 776-1218)

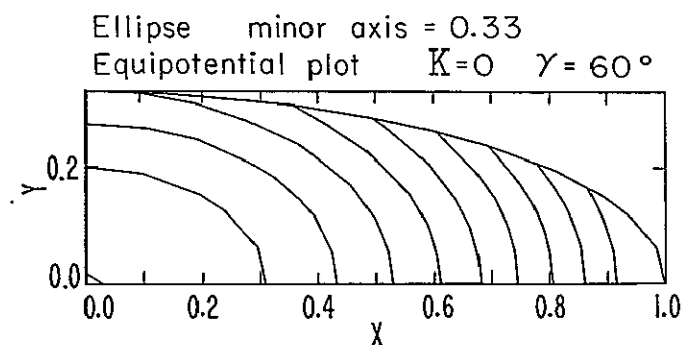


Fig. 8. Level curves of the capillary surface for $\gamma = 60^\circ$, $a = 1.0$, and $b = 0.33$. (XBL 776-1126)

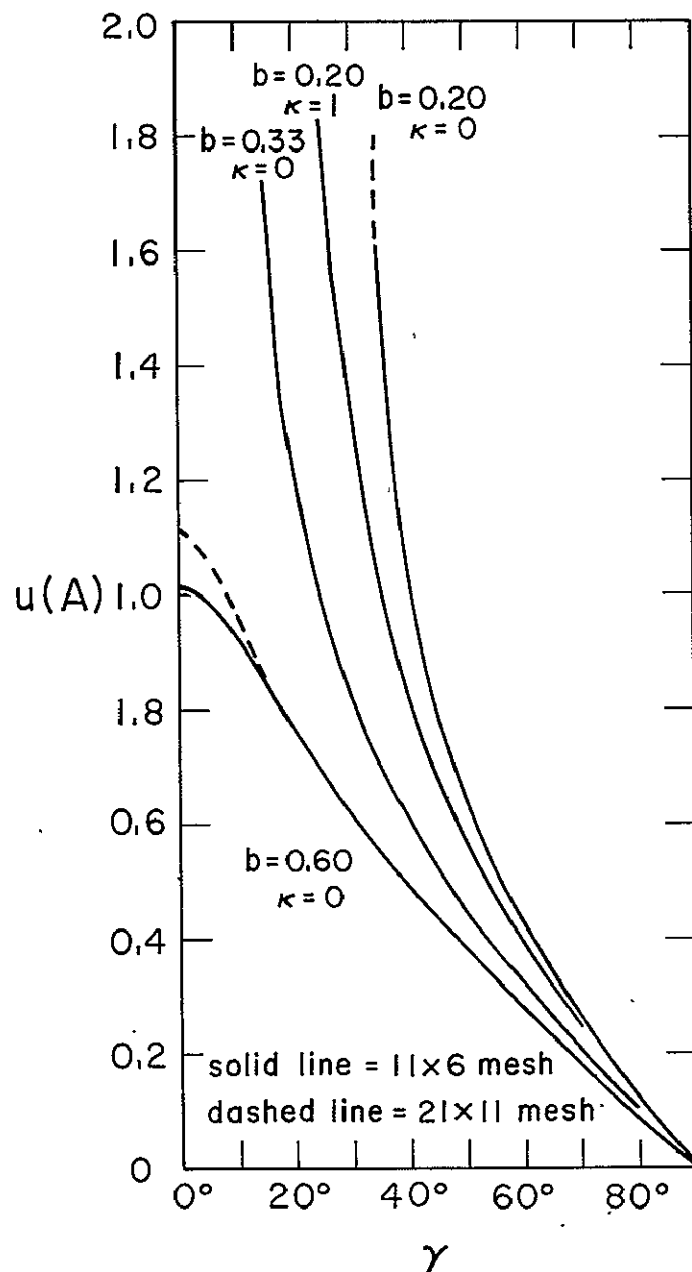


Fig. 9. Height u of the capillary surface at the point A as a function of the contact angle γ for $\kappa = 0$ and $b = 0.60, 0.33$, and 0.20 and for $\kappa = 1$ and $b = 0.20$. (XBL 775-953)

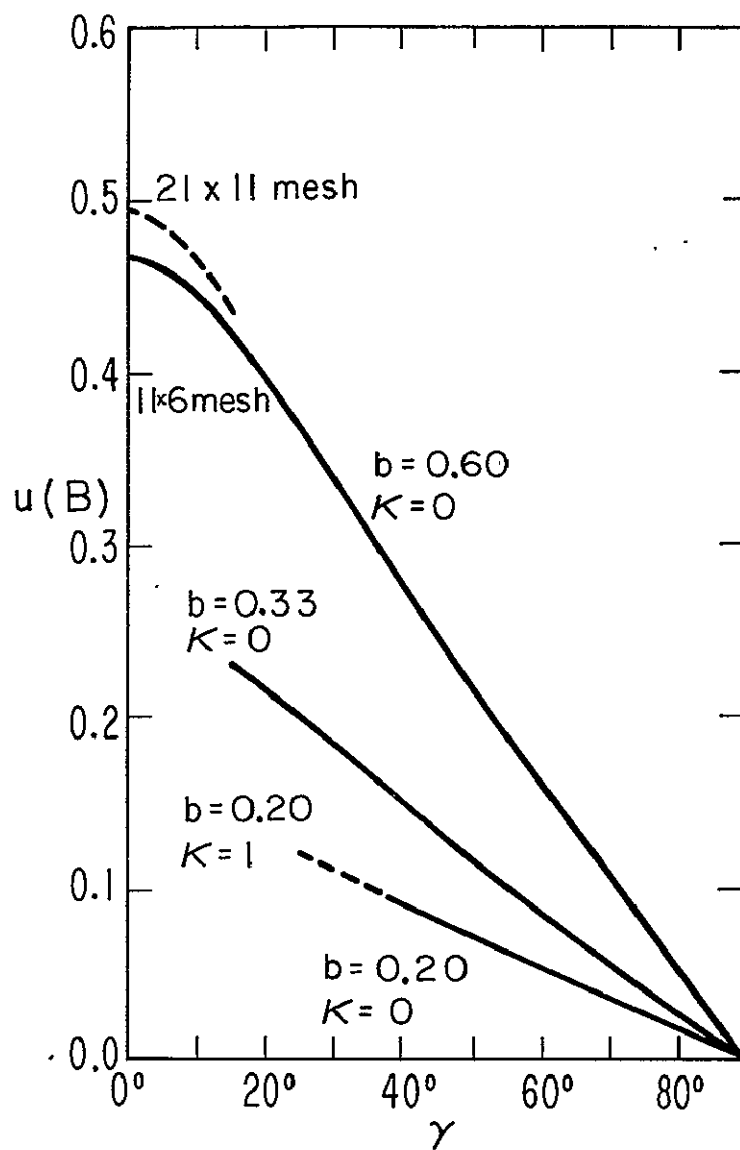


Fig. 10. Height u of the capillary surface at the point B as a function of the contact angle γ for $\kappa = 0$ and $b = 0.60$, 0.33 , and 0.20 and for $\kappa = 1$ and $b = 0.20$. (XBL 776-1118)

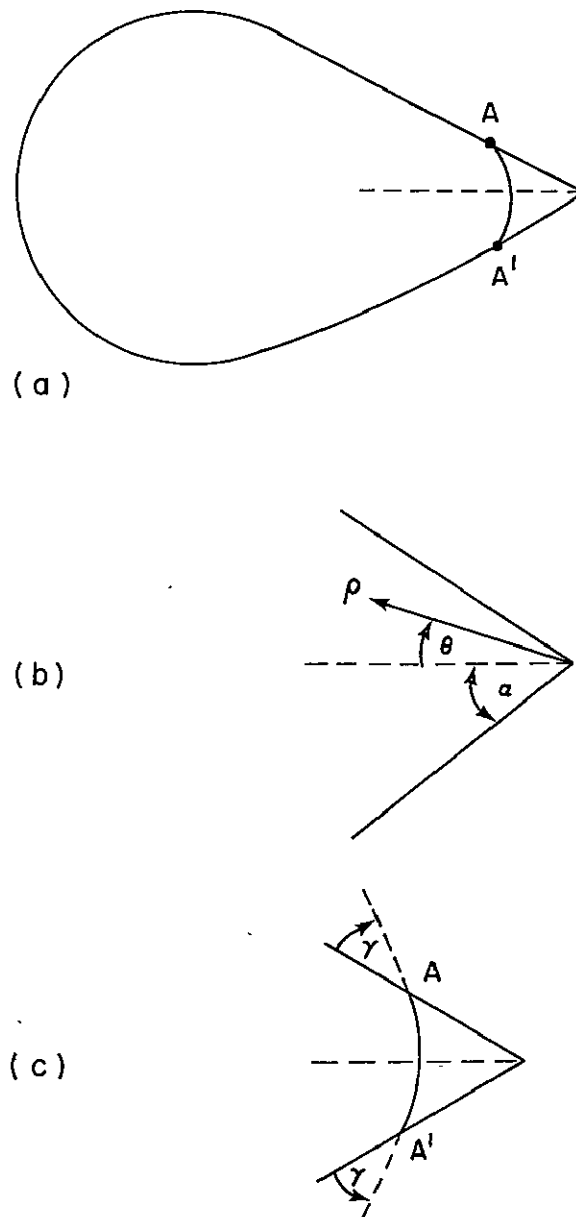


Fig. 11. Cross section of a cylinder and details.

(XBL 775-950)

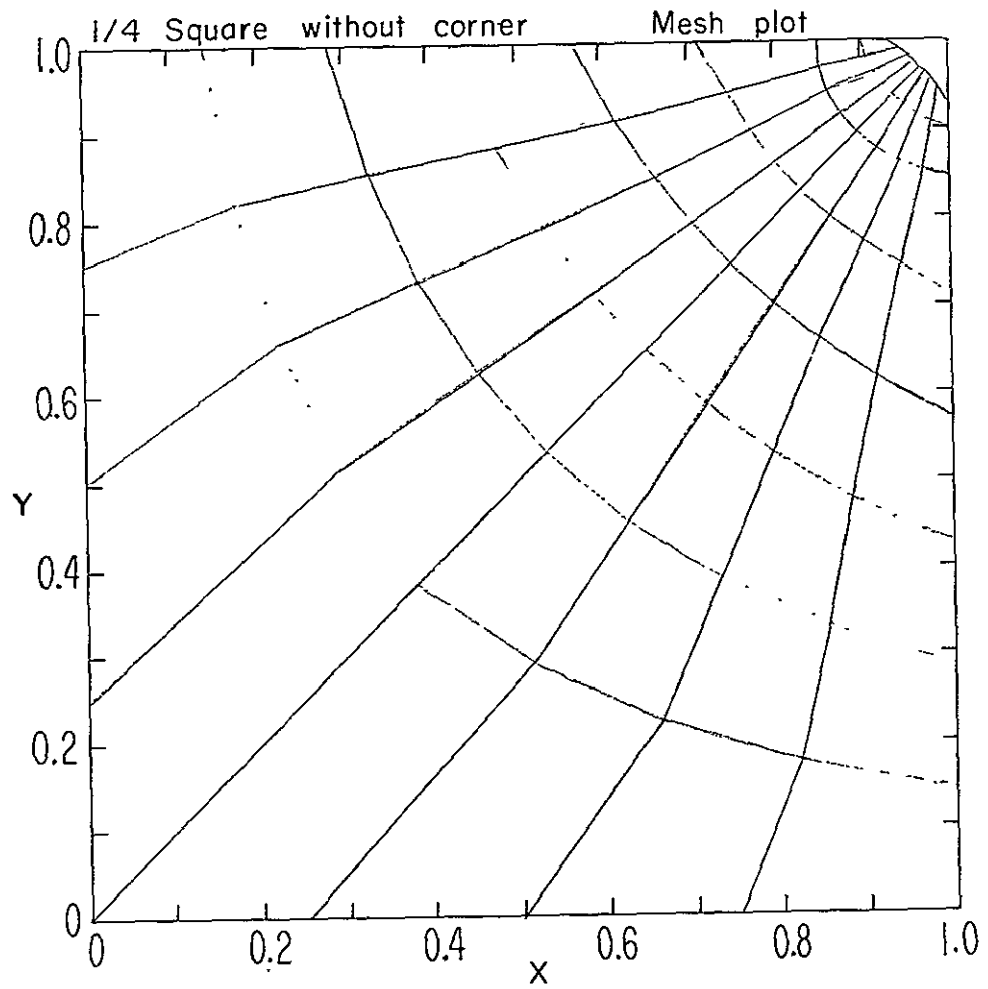


Fig. 12. 9x9 mesh for a 1/4 square with the corner deleted.
(XBL 776-1220)

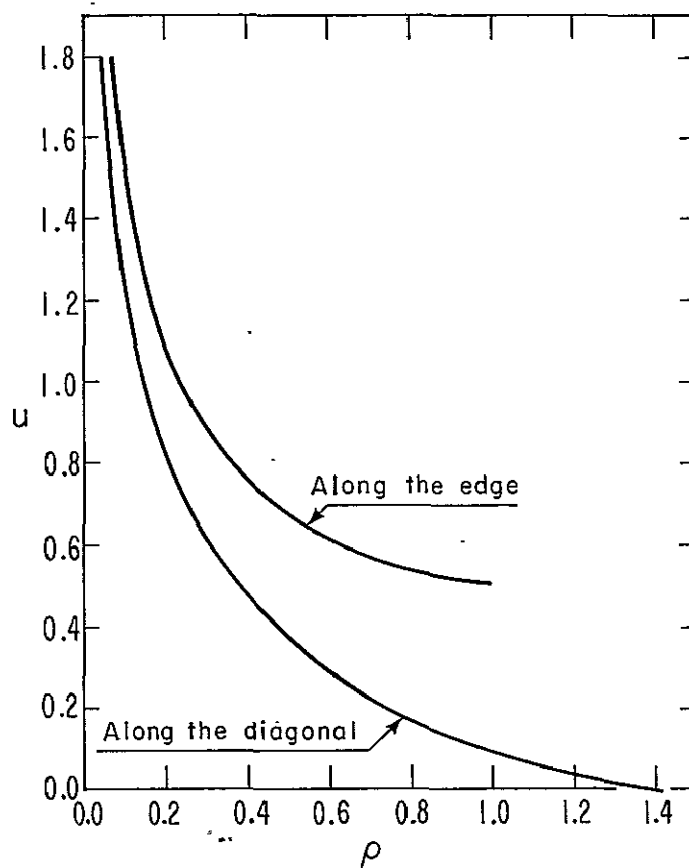


Fig. 13. Height u of the capillary surface along the edge and the diagonal, respectively, as a function of the distance ρ from the corner.
(XBL 776-1120)

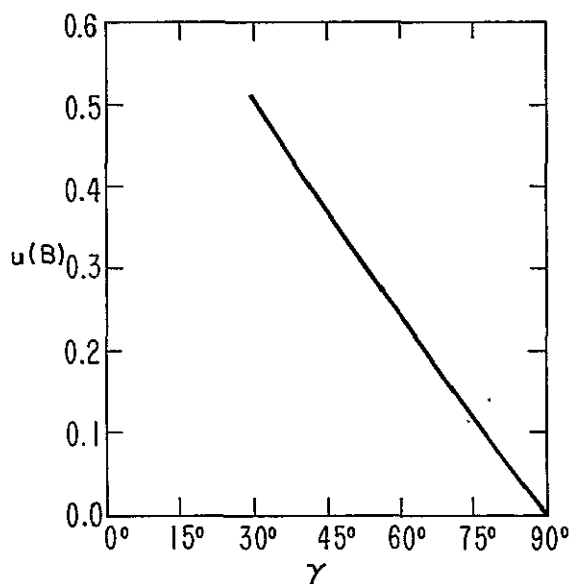


Fig. 14. Height u of the capillary surface at the midpoint B of the edge of the full square as a function of contact angle γ .
(XBL 776-1115)

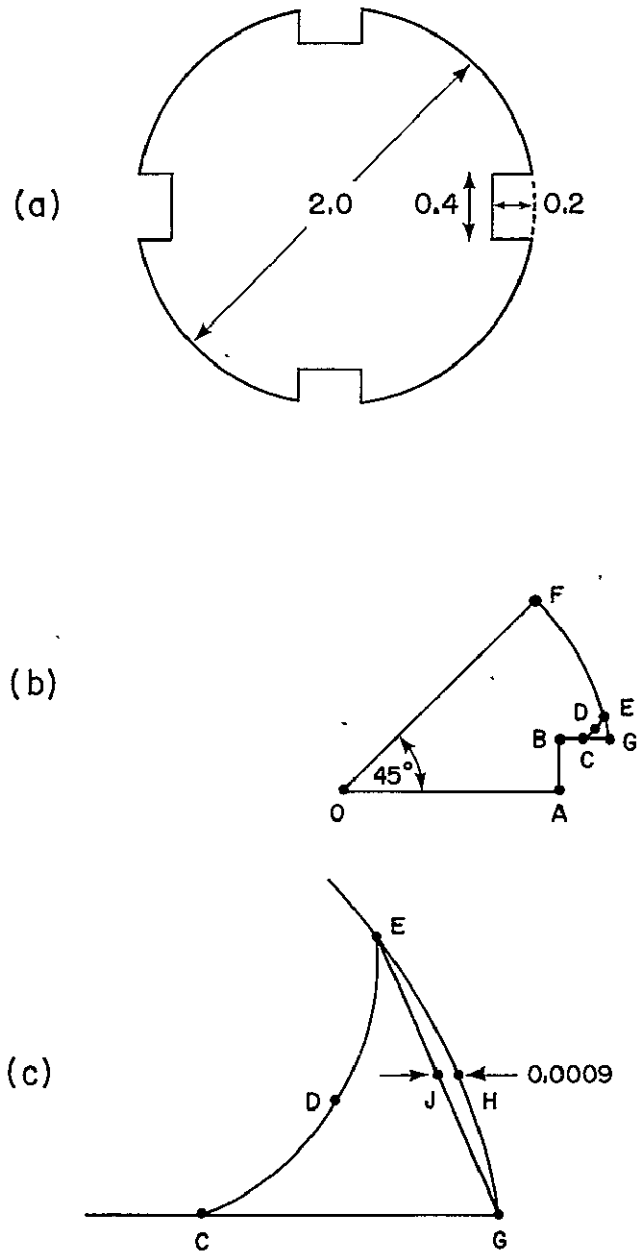


Fig. 15. Cross section of a cylinder with a reentrant notch, and details.
(XBL 775-951)

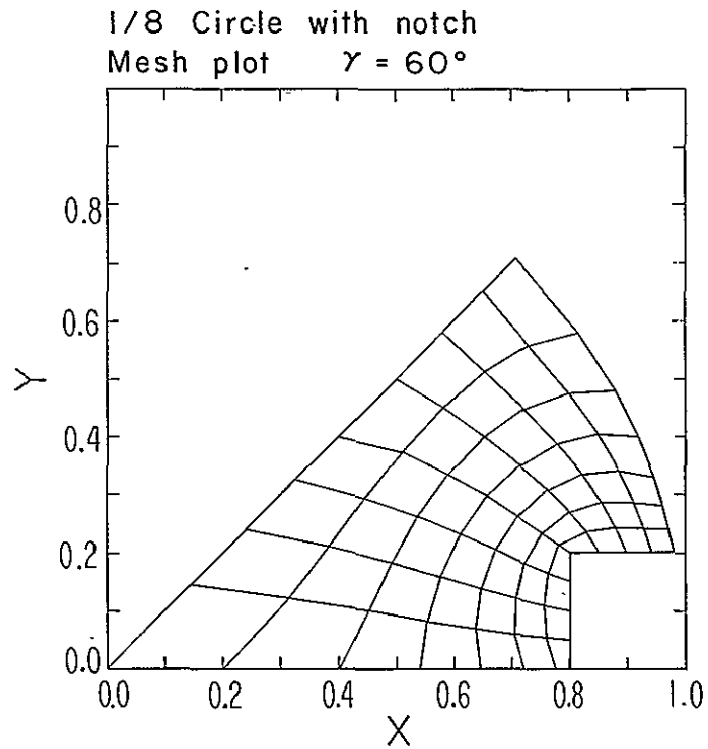


Fig. 16. 9×8 mesh for a cylinder with a reentrant notch for $\gamma = 60^\circ$.
(XBL 776-1123)

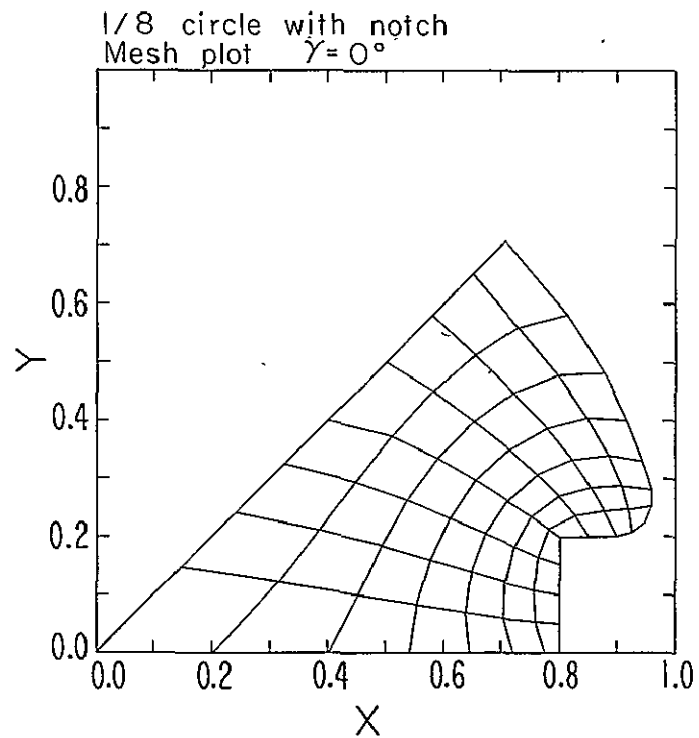


Fig. 17. 9×8 mesh for a cylinder with a reentrant notch for $\gamma = 0^\circ$.
(XBL 776-1122)

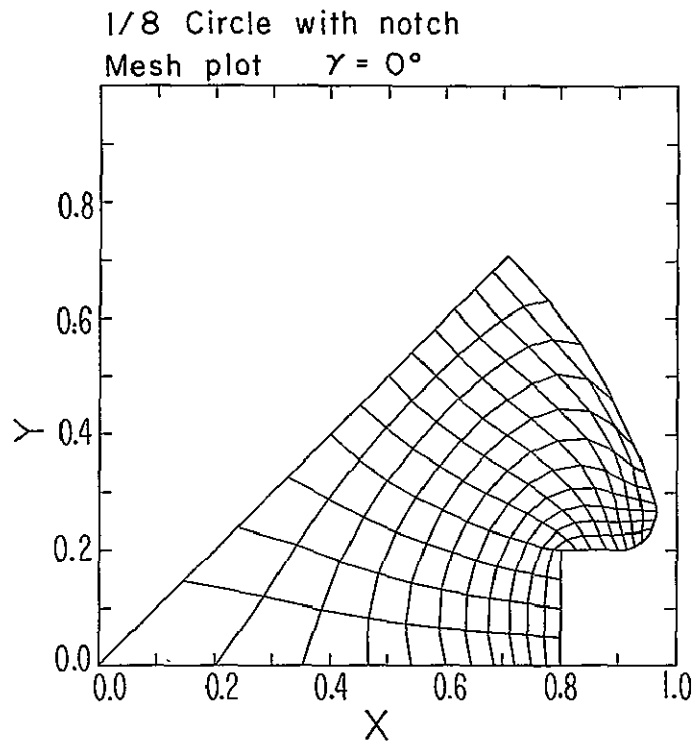


Fig. 18. 13x12 mesh for a cylinder with a reentrant notch for $\gamma = 0^\circ$.
(XBL 776-1125)

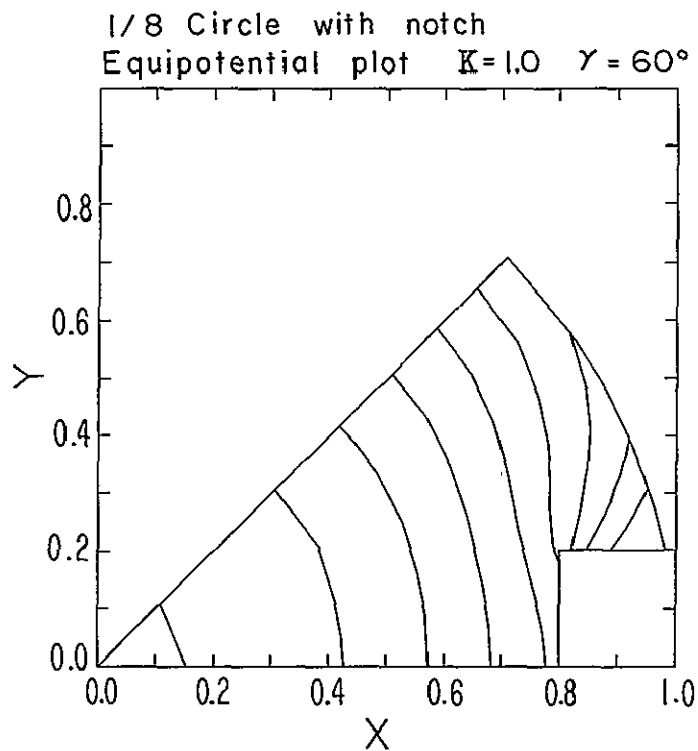


Fig. 19. Level curves of the capillary surface for $\gamma = 60^\circ$.
(XBL 776-1124)

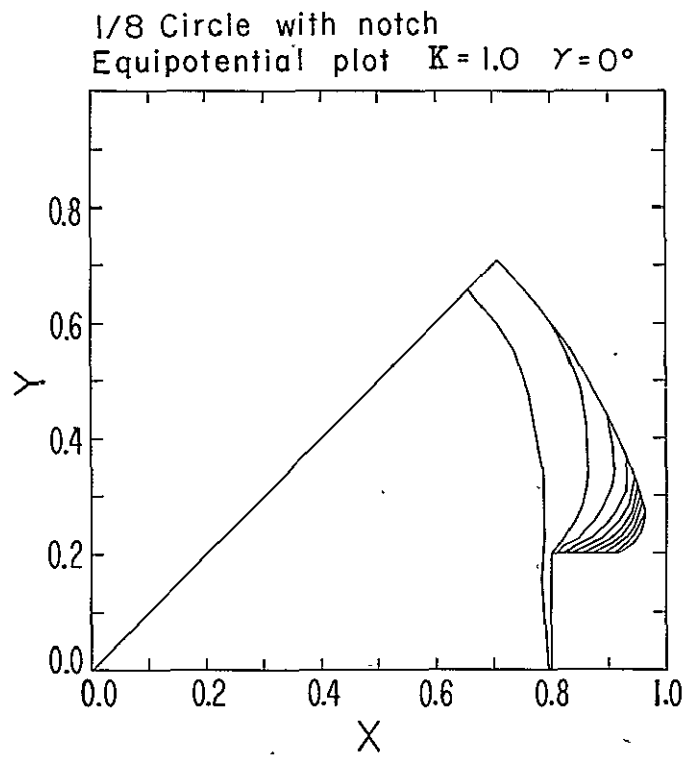


Fig. 20. Level curves of the capillary surface for $\gamma = 0^\circ$.
(XBL 776-1121)

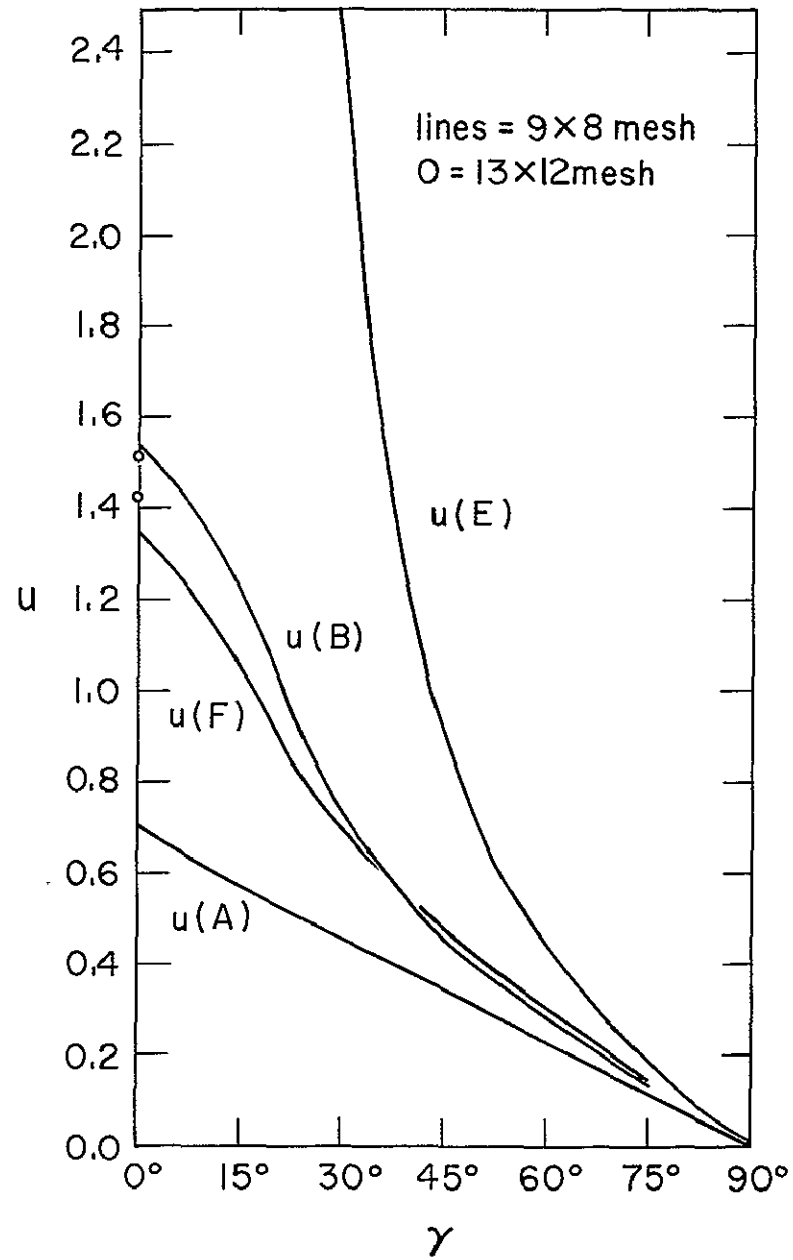


Fig. 21. Height u of the capillary surface at points A, B, E, and F as a function of contact angle γ . (XBL 775-952)

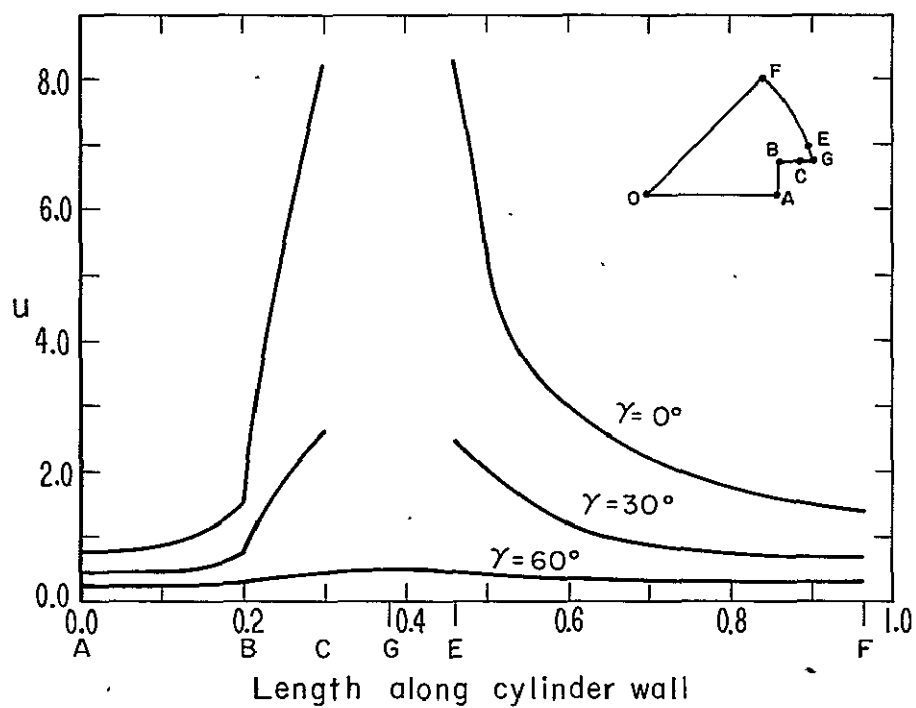


Fig. 22. Height u of the capillary surface as a function of arc length along the cylinder wall for $\gamma = 0^\circ$, 30° , and 60° .
(XBL 776-1119)

APPENDIX V

SOME PROPERTIES OF CAPILLARY SURFACES ON
ELLIPTICAL DOMAINS

by

Norman Albright

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SOME PROPERTIES OF CAPILLARY SURFACES
ON ELLIPTICAL DOMAINS

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ABSTRACT

In this report we show there will exist a critical contact angle for an elliptical cross section if the ratio b/a of the minor and major semiaxes is less than 0.6116. (There is no solution of the capillary surface Eqs. (1) and (2) for contact angles less than the critical angle.) We also calculate a lower bound on γ_{crit} for various values of b/a . These bounds appear to be close to the values of γ_{crit} found by numerical solution of Eqs. (1) and (2).

1. DEFINITION OF THE PROBLEM

We consider the equilibrium free surface of a liquid partly filling a vertical cylinder for the case in which the surface height $u(x,y)$ is a single-valued smooth function of x and y , and in which there is sufficient liquid to cover the base of the cylinder entirely. The gravitational field is taken to be positive when directed vertically downward. The height then satisfies the equation

$$\nabla \cdot \left(\frac{1}{W} \nabla u \right) = \kappa u + 2H \quad (1)$$

$$W = (1 + |\nabla u|^2)^{1/2},$$

where ∇ is the two-dimensional operator $(\partial/\partial x, \partial/\partial y)$, $\kappa = \rho g/\sigma$ is the capillary constant, ρ is the difference in densities between the liquid and gas phases, g is the acceleration due to gravity, and σ is the gas-liquid surface tension. The constant $2H$ is determined by the cross-sectional shape of the cylinder, the volume of liquid, and the boundary condition satisfied by the free surface of the liquid at the cylinder wall.

The boundary condition for a free surface that makes a contact angle γ with the cylinder wall is

$$\frac{1}{W} \frac{\partial u}{\partial n} = \cos \gamma \quad \text{at the wall,} \quad (2)$$

where $\partial u/\partial n$ denotes the derivative of u with respect to the outward directed normal at the wall. Only the case of wetting liquids $0^\circ \leq \gamma < 90^\circ$, will be considered here. (The nonwetting case can be obtained from it directly by means of a simple transformation.)

2. CRITERION FOR THE EXISTENCE OF A CRITICAL CONTACT ANGLE FOR ELLIPTICAL CROSS SECTIONS

Let A denote the area and L the perimeter of the cross section of a cylinder. The following theorem holds [1,2].

Theorem. Suppose there is a point p on the boundary at which the curvature is greater than L/A ; then there exists a critical contact angle such that there is no solution of Eqs. (1) and (2) in a neighborhood of p for $0 \leq \gamma < \gamma_{\text{crit}}$.

We shall apply this theorem to an elliptical cross section. For this application we must calculate the area and perimeter of an ellipse and the curvature at any point on it. The area of an ellipse is

$$A = \pi ab \quad (3)$$

where a and b are the semimajor and semiminor axes.

The ellipse is described by the equation

$$y(x) = b (1 - x^2/a^2)^{1/2} \quad (4)$$

The perimeter of the ellipse is

$$\begin{aligned} L &= 4 \int_0^a [1 + (y')^2]^{1/2} dx \\ &= 4 \int_0^a \frac{[1 - (1 - b^2/a^2) x^2/a^2]^{1/2}}{(1 - x^2/a^2)^{1/2}} dx \end{aligned}$$

Let $x/a = \sin \theta$, and

$$m = 1 - b^2/a^2 \quad (5)$$

Then

$$L = 4aE(m) \quad , \quad (6)$$

where

$$E(m) = \int_0^{\pi/2} (1 - m \sin^2 \theta)^{\frac{1}{2}} d\theta \quad (7)$$

is the complete elliptic integral of the second kind. Values of L/A for $a = 1$ and various values of b are given in Table I to the indicated number of decimal places.

Table I. Values of L/A for $a = 1$ and various values of b .

b	m	L/A
0.2	0.96	6.688
0.25	0.9375	5.461
0.33	0.8911	4.290
0.4	0.84	3.663
0.5	0.75	3.084
0.6	0.64	2.708

These will be used in a later section of this report.

Next we shall calculate the curvature. The differential of arc length is

$$ds = [1 + (y')^2]^{1/2} dx$$

The unit vector $\hat{t}$ tangent to the curve $y(x)$ in two dimensions is

$$\begin{aligned} \hat{t} &= (dx/ds, dy/ds) \\ &= [1 + (y')^2]^{-1/2} (1, y') \end{aligned} \quad (8)$$

The curvature C and the unit vector $\hat{n}$ normal to the curve $y(x)$ are defined by

$$\begin{aligned} C\hat{n} &= d\hat{t}/ds \\ d\hat{t}/ds &= [1 + (y')^2]^{-1/2} d\hat{t}/dx \\ &= y'' [1 + (y')^2]^{-2} (-y', 1) . \end{aligned} \quad (9)$$

Therefore

$$\hat{n} = \text{sgn}(y'') [1 + (y')^2]^{-1/2} (-y', 1) \quad (10)$$

and

$$C = |y'' [1 + (y')^2]^{-3/2}| . \quad (11)$$

Note that C also can be written

$$C = \left| \frac{d}{dx} \left\{ y' [1 + (y')^2]^{1/2} \right\} \right| . \quad (12)$$

Let $y(x)$ be an ellipse. Then

$$y' = -b^2 x / a^2 y$$

$$y'' = -b^4 / a^2 y^3$$

Thus

$$C = a^4 b^4 / (a^4 y^2 + b^4 x^2)^{3/2}$$

The curvature is maximum at the point $x = a, y = 0$ where the major axis intersects the ellipse. Thus

$$C_{\max} = a/b^2 . \quad (13)$$

According to the theorem, there will exist a critical contact angle for ellipses with $C_{\max}$ greater than L/A , that is, for

$$b/a < \pi/4E(m) . \quad (14)$$

This inequality can be solved numerically. The result is that a critical angle will exist for ellipses with $b/a < 0.6116$.

3. A LOWER BOUND ON γ_{crit}

Consider the cross section of the cylinder shown in Fig. 1. Let A be the area of the entire cross section and L be its perimeter. The cross section is cut by a curve Γ , which intersects the perimeter at points p_1 and p_2 , and whose length we also denote by Γ . Let A^* denote the part of the domain cut off by Γ and denote also the area of this part. Let L^* denote the part of the perimeter cut off by Γ and denote also the length of this part.

If a solution to Eqs. (1) and (2) exists for $\kappa = 0$ and contact angle γ , then integration of Eq. (1) over A^* gives

$$\begin{aligned} 2HA^* &= \int_{A^*} \nabla \cdot \left(\frac{1}{W} \nabla u \right) dA = \int_{\Gamma+L^*} \left(\frac{1}{W} \nabla u \right) \cdot \hat{n} dL \\ &= L^* \cos \gamma + \int_{\Gamma} \left(\frac{1}{W} \nabla u \right) \cdot \hat{n} dL . \end{aligned}$$

Now $|\hat{n} \cdot \nabla u| \leq |\nabla u| \leq W$; therefore

$$-\Gamma \leq \int_{\Gamma} \left(\frac{1}{W} \nabla u \right) \cdot \hat{n} dL \leq \Gamma .$$

Thus if a solution exists for contact angle γ , then for any curve Γ

$$-\Gamma \leq 2HA^* - L^* \cos \gamma \leq \Gamma . \quad (15)$$

This can be written

$$\frac{2HA^* - \Gamma}{L^*} \leq \cos \gamma \leq \frac{2HA^* + \Gamma}{L^*} . \quad (16)$$

Integration of Eq. (1) over the entire cross section gives

$$2HA = L \cos \gamma .$$

Eliminating H from Eq. (15) gives

$$-\Gamma \leq (L^* - A^*L/A) \cos \gamma \leq \Gamma .$$

For $0 \leq \gamma \leq 90^\circ$ and $L^* - A^*L/A$ nonzero, this can be written

$$\cos \gamma \leq V , \quad (17)$$

where

$$V = \frac{\Gamma}{|L^* - A^*L/A|} . \quad (18)$$

Equations (16) and (17) are Lemma 6 and Corollary 3.2 of Ref. 2 for the special case of a two-dimensional domain.

Equation (17) holds for each contact angle for which a solution to Eqs. (1) and (2) exists. In particular it holds for γ_{crit} . Let V_0 be the minimum of V with respect to all possible curves Γ . V_0 is an upper bound for $\cos \gamma_{\text{crit}}$.

$$\cos \gamma_{\text{crit}} \leq V_0 . \quad (19)$$

This gives a lower bound on γ_{crit} .

4. MINIMIZATION OF V FOR FIXED p_1 AND p_2

The minimization of V can be done in two steps. First, find Γ that minimizes V for a fixed pair of intersection points p_1 and p_2 ; then vary p_1 and p_2 . It can be shown that the minimizing Γ is the arc of a circle [2].

Let R be the radius of the circular arc Γ , and let O be the center of the circle as shown in Fig. 2. Let $2y$ be the length of the chord from p_1 to p_2 . Let A be the area of the region bounded by this chord and by Γ . Let 2θ be the angle $p_1 O p_2$. Then the following relations hold.

$$\theta = \arcsin (y/R) \quad (20)$$

$$\Gamma = 2R\theta \quad (21)$$

$$A_1 = R^2\theta - yR \cos \theta \quad (22)$$

Let us hold p_1 and p_2 fixed and vary R . Then y is fixed, but θ , Γ , and A_1 vary. Also $\delta A^* = -\delta A_1$ because $A^* + A_1$ is fixed.

Varying R in Eqs. (20)-(22) and eliminating $\delta\theta$ gives

$$\delta\Gamma = 2(\theta - \tan \theta) \delta R$$

$$\delta A^* = -2R(\theta - \tan \theta) \delta R$$

thus

$$\delta A^* = -R \delta\Gamma. \quad (23)$$

Let $(L^* - A^*L/A)$ be positive; then

$$(L^* - A^*L/A) \delta V = \delta\Gamma + (VL/A) \delta A^* \quad (24)$$

Let V_p be the minimum value of V for fixed points p_1 and p_2 , and let R_p be the minimizing radius. Setting $\delta V = 0$ in Eq. (24) and using Eq. (23) gives

$$R_p = A/(LV_p) \quad (25)$$

5. MINIMIZATION OF V WITH p_1 AND p_2

Next, let us hold R fixed and vary p_1 and p_2 . Let ϕ_1 denote the acute angle of intersection of Γ with the cross section at p_1 , and let ϕ_2 denote the corresponding angle at p_2 . Let δL_1^* be the variation in L^* at p_1 , and δL_2^* be the variation at p_2 . Then

$$\delta\Gamma = \cos \phi_1 \delta L_1^* + \cos \phi_2 \delta L_2^* \quad (26)$$

$$\delta A^* = (\Gamma/2) \sin \phi_1 \delta L_1^* + (\Gamma/2) \sin \phi_2 \delta L_2^* \quad (27)$$

Let $(L^* - A^*L/A)$ be positive; then

$$(L^* - A^*L/A) \delta V = \delta \Gamma + (VL/A) \delta A^* - V \delta L^* \quad (28)$$

Setting $\delta V = 0$ in Eq. (28) and using Eqs. (26) and (27) gives two equations for the coefficients of the independent variations δL_1^* and δL_2^* .

$$\cos \phi_1 + U \sin \phi_1 = V \quad (29)$$

$$\cos \phi_2 + U \sin \phi_2 = V, \quad (30)$$

where

$$U = VL\Gamma/2A$$

For a given value of V , L , Γ , and A , Eq. (29) has the solutions

$$\sin \phi_1 = \left\{ U \pm [U^2 + (1 + U^2)(1 - V^2)]^{1/2} \right\} / (1 + U^2).$$

For $V < 1$, Eq. (29) has one positive solution for $\sin \phi_1$. For $V > 1$, it has two positive solutions; however, $V > 1$ gives no useful bound on $\cos \gamma_{\text{crit}}$, so we shall ignore this case. Thus if V has a relative minimum that is less than one, then ϕ_1 will equal ϕ_2 for the minimizing Γ .

Consider a cross section that is symmetric about some straight line, as is the ellipse of Fig. 3 about the x axis. Let the curve Γ have intersection points p_1 and p_2 on opposite sides of that line. If V has a relative minimum that is less than one, then the minimizing p_1 and p_2 will be symmetric about that line.

6. LOWER BOUND ON γ_{crit} FOR ELLIPTICAL CROSS SECTIONS

We apply the preceding results to the elliptical cross section shown in Fig. 3. The ellipse is

$$y(x) = b(1 - x^2/a^2)^{1/2} . \quad (31)$$

Let p_1 be the point $[x_1, y(x_1)]$; it is sufficient to take p_2 to be $[x_1, -y(x_1)]$. Let A_2 be the area $A_1 + A^*$; then

$$A_2 = 2 \int_{x_1}^a y(x) dx \quad (32)$$

$$A^* = A_2 - A_1 \quad (33)$$

$$L^* = 2 \int_{x_1}^a [1 + (y')^2]^{1/2} dx . \quad (34)$$

Equations (18), (20)-(22), (25), and (31)-(34) can be solved for V_p for each value of x_1 . By calculating V_p for a sequence of values of x_1 , we find the minimum value V_0 .

The circular arc Γ must lie inside the ellipse. This is assured if R is greater than R_1 . R_1 is the length of the line $O_1 p_1$ that is perpendicular to the ellipse at p_1 as shown in Fig. 3.

$$R_1^2 = [y(x_1)]^2 + b^4 x_1^2 / a^4 \quad (35)$$

$$R = \max(R_1, R_p) . \quad (36)$$

The preceding equations give the following results for the lower bound on γ_{crit} for $a = 1$ and various values of b .

b	lower bound
0.20	35.12°
0.25	26.95°
0.33	16.88°
0.40	10.32°
0.50	3.71°
0.60	0.12°

These bounds appear to be close to the values of γ_{crit} found by numerical solution of Eqs. (1) and (2) [3]. The lower bound as a function of b is shown in Fig. 4.

ACKNOWLEDGMENTS

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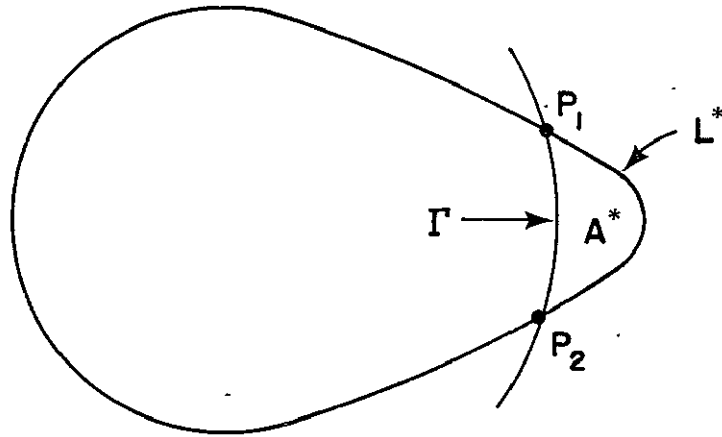


Fig. 1. Cross section of a cylinder. (XBL 776-949)

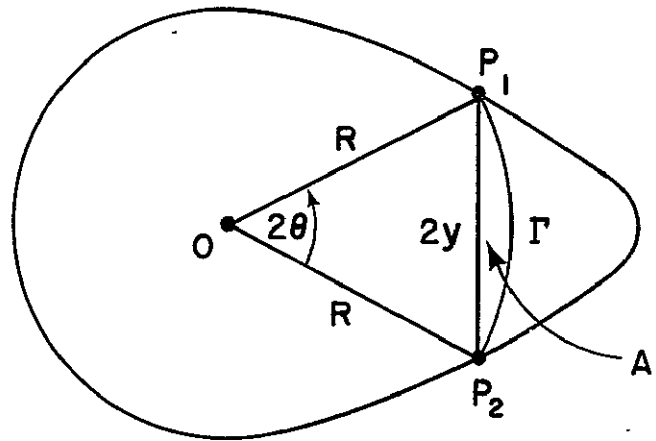


Fig. 2. Cross section of a cylinder with variables defined. (XBL 776-949)

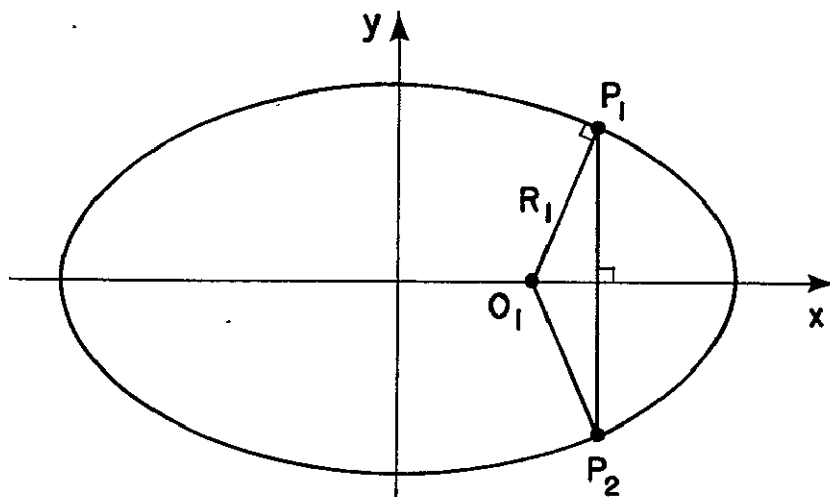


Fig. 3. Cross section of an ellipse. (XBL 776-949)

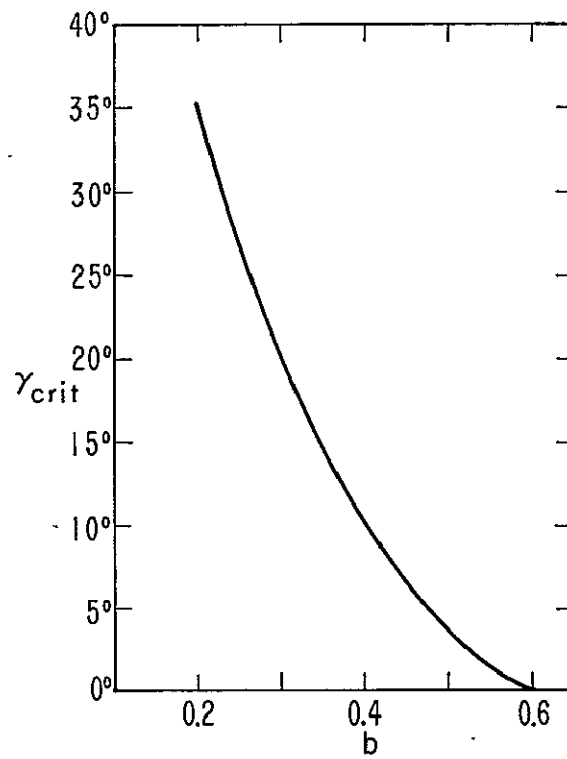


Fig. 4. Lower bound on γ_{crit} as a function of the ratio b of the semiminor and semimajor axes. (XBL 776-1117)

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16. Abstract The results of several independent studies are presented. In the first, the general question is considered of whether a wetting liquid always rises higher in a small capillary tube than in a larger one, when both are dipped vertically into an infinite reservoir. It is proved, by example, that the answer in some cases is negative. In the second study, an analytical investigation is initiated to determine the qualitative behavior of the family of solutions of the equilibrium capillary free-surface equation that correspond to rotationally symmetric pendent liquid drops and the relationship of these solutions to the singular solution, which corresponds to an infinite spike of liquid extending downward to infinity. The next two studies are computational ones. In the first the block successive overrelaxation-Newton method and the generalized conjugate gradient method are investigated for solving the capillary equation on a uniform square mesh in a square domain, including the case for which the solution is unbounded at the corners. In the second, capillary surfaces are calculated on the ellipse, on a circle with reentrant notches, and on other irregularly shaped domains using JASON, a general-purpose program for solving nonlinear elliptic equations on a nonuniform quadrilateral mesh. In the last study, analytical estimates for the nonexistence of solutions of the equilibrium capillary free-surface equation on the ellipse in zero gravity are evaluated.					
17. Key Words (Suggested by Author(s)) Liquid-vapor inter- faces; capillary tubes; drops (liquids); inter- face stability; weightlessness; reduced gravity; analysis (mathematics); existence theorems; numerical analysis; differential equations; finite element method; conjugate gradient method; iteration; nonlinear equations				18. Distribution Statement Unclassified - unlimited STAR Category 34 DOE Category UC-32	
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